DE LA RECHERCHE À L'INDUSTRIE

A Staggered Mimetic ALE Scheme for Hydrodynamics (SMASH) ensuring geometric and energetic consistency

Thibaud Vazquez-Gonzalez[1]
Antoine Llor[1] and Christophe Fochesato[1]

[1] CEA, DAM, DIF, F-91297 Arpajon, France,

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Outline

- Scientific context : ALE schemes and numerial mimetism
- Discrete derivation of the scheme
  - Discretization of fields and transport
  - Discrete action integral and Euler–Lagrange equations
  - Global strategy of derivation
  - Main steps of scheme
- Numerical tests
  - 1D indifference to implicit–explicit advection
  - 2D indifference to grid motion strategy
  - 1D–2D versatility in the choice of grid velocity
- Conclusions and perspectives

Scientific context

Simulation of applied, non-stationnary, and compressible single-fluid flows (shocks and grid deformations)
The numerical scheme must comply with several constraints :

- Arbitrary evolution of the computational domain and grid
- Exact conservation of mass, momentum and total energy
- Thermodynamically consistent capture of pressure work (hence entropy)
- Robustness and stability in presence of shocks and mesh deformations
- Compatibility with other physics and competing stiff phenomena

Usually, simulation of continuum dynamics use Eulerian or Lagrangian reference frames

- Eulerian : simulations on fixed grids $\longrightarrow$ stable and robust results but diffusive schemes
- Lagrangian : grids evolve with material velocities $\longrightarrow$ less diffusive but critical grid distortions when simulating realistic flows

These combined features have encouraged the use of ALE (Arbitrary Lagrangian Eulerian) methods in CFD.

ALE methods

Two main types of ALE approaches

- Indirect ALE : coupling a Lagrangian evolution phase to a remapping procedure after each or several time steps
  $\hookrightarrow$ results more robust and less diffusive but conservation issues in staggered mesh and computational cost of remapping in 2–3D
- Direct ALE : grid subjected to arbitrary motions
  $\hookrightarrow$ mass, momentum, and energy fluxes are taken into account directly in the discrete evolution equations
  $\hookrightarrow$ grid node velocities are given a priori (user defined), and possibly constraint by boundary conditions, Lagrangian limit, tracking of characteristics, etc ...

Mimetic schemes

Application of least action principle to discrete action integral

- Special case of broad class of numerical mimetism : transposing as accurately as possible some critically important physical constraints into discrete equations
- Use of mimicking schemes rather limited in CFD
  $\hookrightarrow$ non-holonomic constraints with mass and entropy advections and non-symetric form of discrete Lagrangian can lead to non-conservative evolution equations
- However, application of least action principle is well motivated in CFD
  - Capture of the pressure work done in a thermodynamical consistent way
  - Derivation using only algebraic quantities instead of the usual PDEs
  - Yields powerful numerical schemes for long time integrations when applied to Hamiltonian systems

Reminders on the least action principle :

- Start from continuous Lagrangian of hydrodynamics :
  $\mathcal{L} = \frac{1}{2}\rho\mu_i\mu_i - \rho e(\rho) + \phi[\partial_t\rho + (\rho u_i)_{,i})]$
- Application of least action principle $\delta\mathcal{A} = \iint \left[\frac{\partial\mathcal{L}}{\partial\phi}\delta\phi + \frac{\partial\mathcal{L}}{\partial u_i}\delta u_i + \frac{\partial\mathcal{L}}{\partial\rho}\delta\rho\right] d^3\mathbf{x}dt$
- Evolution equations for mass and momentum in the local grid frame

$$\partial_t\rho + (\rho u_i)_{,i} = 0 \ , \tag{1a}$$
$$\partial_t(\rho\mu_i) + (\rho\mu_i u_j)_{,j} = -P_{,i} \tag{1b}$$

where $\mathbf{w}$, $\mathbf{u}$ and $\boldsymbol{\mu} = \mathbf{u} + \mathbf{w}$ are resp. grid velocity, relative velocity and absolute velocity

Present approach

The approach developped here tends to regroup

- Direct ALE formalism $\longrightarrow$ robustness and stability in presence of strong shocks and deformations
- Least action principle $\longrightarrow$ thermodynamically consistent capture of pressure work

Similar combinaisons already tested :

- ALE + LAP $\longrightarrow$ [Koo, 2000]
- Incomp. Euler + symplectic LAP $\longrightarrow$ [Pavlov, 2011]

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Space and time localisations of thermodynamic quantities and velocities

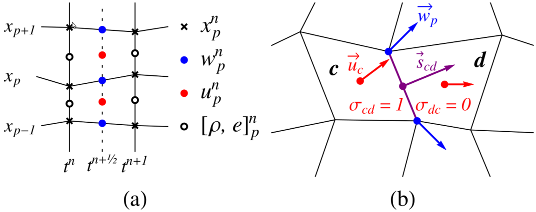


FIGURE: (a) 1D representation of a space-time element with the localisation of thermodynamic quantities and velocities ; (b) Space localisation of grid and relative-to-grid velocities, and of the corresponding upwinding coefficients.

Notations :

- $\mathbf{w}$ grid velocity
- $\mathbf{u}$ fluid velocity relative to the grid
- $\boldsymbol{\mu} = \mathbf{u} + \mathbf{w}$ absolute velocity of the fluid
- $\mathbf{s}_{cd}^n$ outward pointing vector to boundary between c—d (magnitude given by the area of the c–d)
- $\sigma_{cd}^{n+1/2} = \frac{1}{2}\left[1 + \mathrm{sign}(\mathbf{s}_{cd}^{n+1/2} \cdot \mathbf{u}_c^{n+1/2})\right]$ off-centering factor of transport from c to d
- ρ and e resp. density and internal energy
- $\Delta t^{n+1/2} = t^{n+1} - t^n$ time step between t^n and t^{n+1}

Internal energy

$$\iint \rho e(\rho)\, d^3\mathbf{x}dt \rightsquigarrow \sum_n \sum_c \Delta t^n V_c^n \rho_c^n e_c^n \ . \tag{2}$$

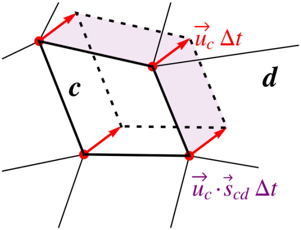
Kinetic energy

$$\iint \tfrac{1}{2}\rho(u_i + w_i)^2\, d^3\mathbf{x}dt \rightsquigarrow \sum_n \sum_c \Delta t^{n-1/2} V_c^n \,\tfrac{1}{2}\, \rho_c^n (\boldsymbol{\mu}_c^{n-1/2})^2 \ . \tag{3}$$

Remarks :

- $\Delta t^n = \frac{1}{2}(\Delta t^{n+1/2} + \Delta t^{n-1/2})$
- $\boldsymbol{\mu}_c^{n+1/2} = \mathbf{u}_c^{n+1/2} + \mathbf{w}_c^{n+1/2}$ with $\mathbf{w}_c^{n+1/2} = \frac{1}{|\mathcal{P}(c)|}\sum_{\mathcal{P}(c)} \mathbf{w}_p^{n+1/2}$
- $\boldsymbol{\mu}_c^{n-1/2}$ is $\Delta t^{n-1/2}/2$ behind density ρ_c^n allows to factorize ρ_c^n when obtaining the discrete absolute velocity equation
- Full midpoint rule in time in the Lagrangian limit as $V_c^n \rho_c^n = V_c^{n+1/2} \rho_c^{n+1/2}$

Discretization of mass transport



$$V_c^{n+1}\rho_c^{n+1} - V_c^n\rho_c^n - \Delta t^{n+1/2} \sum_{d\in\mathcal{D}(c)} \left(\sigma_{dc}^{n+1/2}\mathbf{s}_{dc}^{n+1/2}\cdot\mathbf{u}_d^{n+1/2}\rho_d^{n+1} - \sigma_{cd}^{n+1/2}\mathbf{s}_{cd}^{n+1/2}\cdot\mathbf{u}_c^{n+1/2}\rho_c^{n+1}\right) = 0\,. \quad (4)$$

Remarks on (4) :

- Simple first-order-in-space-and-time upwind scheme for the computation of the mass fluxes between cell c and d
- ρ must be $\Delta t^{n-1/2}/2$ ahead of $\boldsymbol{\mu}$ as already observed for Ec
  $\hookrightarrow$ implicit mass transport but explicit absolute velocity equation
- Mass transport as a rudimentary version of Lagrange plus remap approaches
- 1st accuracy is not incompatible with 2nd order of Ei and Ec but acceptable as a starting point
  $\hookrightarrow$ motion relative to the grid only a correction over the motion captured by the grid

Discrete action integral and variational equations

Discrete action integral of the system

$$\mathcal{A} = \sum_n \sum_c \Bigg\{ \Delta t^{n-1/2} V_c^n \, \tfrac{1}{2} \, \rho_c^n (\boldsymbol{\mu}_c^{n-1/2})^2 - \Delta t^n V_c^n \rho_c^n e_c^n$$

$$+\phi_c^{n+1/2} \Big[V_c^{n+1} \rho_c^{n+1} - V_c^n \rho_c^n - \Delta t^{n+1/2} \sum_{d \in \mathcal{D}(c)} \big(\sigma_{dc}^{n+1/2} \mathbf{s}_{dc}^{n+1/2} \cdot \mathbf{u}_d^{n+1/2} \rho_d^{n+1} - \sigma_{cd}^{n+1/2} \mathbf{s}_{cd}^{n+1/2} \cdot \mathbf{u}_c^{n+1/2} \rho_c^{n+1} \big) \Big] \Bigg\} \, .$$

with the least action principle

$$\delta \mathcal{A} = \sum_n \sum_c \Big(\frac{\partial \mathcal{A}}{\partial \phi_c^{n+1/2}} \delta \phi_c^{n+1/2} + \frac{\partial \mathcal{A}}{\partial \mathbf{u}_c^{n-1/2}} \cdot \delta \mathbf{u}_c^{n-1/2} + \frac{\partial \mathcal{A}}{\partial \rho_c^n} \delta \rho_c^n \Big) = 0 \, . \tag{5}$$

yields the discrete Euler–Lagrange equations

$$V_c^{n+1} \rho_c^{n+1} - V_c^n \rho_c^n + \Delta t^{n+1/2} \sum_{d \in \mathcal{D}(c)} \big(\sigma_{cd}^{n+1/2} \mathbf{s}_{cd}^{n+1/2} \cdot \mathbf{u}_c^{n+1/2} \rho_c^{n+1} - \sigma_{dc}^{n+1/2} \mathbf{s}_{dc}^{n+1/2} \cdot \mathbf{u}_d^{n+1/2} \rho_d^{n+1} \big) = 0 \, ,$$

$$V_c^n \boldsymbol{\mu}_c^{n-1/2} = \sum_{d \in \mathcal{D}(c)} \sigma_{cd}^{n-1/2} \mathbf{s}_{cd}^{n-1/2} \big(\phi_d^{n-1/2} - \phi_c^{n-1/2} \big) \, ,$$

$$\phi_c^{n+1/2} - \phi_c^{n-1/2} = -\Delta t^n \big(e_c^n + P_c^n / \rho_c^n \big) - \Delta t^{n-1/2} \, \tfrac{1}{2} \, \big((\mathbf{u}_c^{n-1/2})^2 - (\mathbf{w}_c^{n-1/2})^2 \big) \, .$$

Global strategy of the discrete derivation

The numerical scheme must respect several important properties

- Elimination of Lagrange multiplier ϕ
- Fully conservative in mass, momentum and total energy
- Only pressure forces are retained
- Explicit evolution of absolute velocity equation (or at least linearly implicit)

In order to preserve these properties, the global strategy of this work is

- Cancel discrete numerical residues at the scheme's order (i.e. 2nd order in Lagrangian limit but only 1st order in Eulerian limit)
- Introduction of so-called time flux terms [CSTS, submitted] when necessary
- Correction of evolution equations as close as possible to the variational equations
- Internal energy equation derived from conservation of total energy
  $\hookrightarrow$ only physical and residual fluxes are left when summing kinetic and internal energies

Main steps of the linearly implicit numerical scheme iSMASH

1) Explicit evolution of absolute velocity

$$V_c^n \rho_c^n (\boldsymbol{\mu}_c^{n+1/2} - \boldsymbol{\mu}_c^{n-1/2}) = -\Delta t^n \sum_{d \in \mathcal{D}(c)} \tfrac{1}{2}(1 + \sigma_{cd}^{n-1/2} - \sigma_{dc}^{n-1/2})\mathbf{s}_{cd}^{n-1/2} (P_d^n - P_c^n)$$
$$+ \Delta t^{n-1/2} \sum_{d \in \mathcal{D}(c)} \sigma_{dc}^{n-1/2} \mathbf{s}_{dc}^{n-1/2} \cdot \mathbf{u}_d^{n-1/2} \rho_d^n \, (\boldsymbol{\mu}_d^{n-1/2} - \boldsymbol{\mu}_c^{n-1/2}) \, . \qquad (7)$$

2) Choice of a grid velocity $\mathbf{w}_p^{n+1/2}$

3) Linearly implicit evolution of mass transport

$$V_c^{n+1}\rho_c^{n+1} - V_c^n \rho_c^n = \Delta t^{n+1/2} \sum_{d \in \mathcal{D}(c)} (\sigma_{dc}^{n+1/2} \mathbf{s}_{dc}^{n+1/2} \cdot \mathbf{u}_d^{n+1/2} \rho_d^{n+1} - \sigma_{cd}^{n+1/2} \mathbf{s}_{cd}^{n+1/2} \cdot \mathbf{u}_c^{n+1/2} \rho_c^{n+1}) \qquad (8)$$

4) Linearly implicit evolution of internal energy

$$V_c^{n+1}\rho_c^{n+1} e_c^{n+1/2} - V_c^n \rho_c^n e_c^n = -\tfrac{1}{2}\Delta t^{n+1/2} [P+Q]_c^n \langle \nabla \cdot \boldsymbol{\mu} \rangle_c^{n+1/4} - \frac{(\Delta t^{n+1/2} - \Delta t^{n-1/2})}{4} [P+Q]_c^n (\langle \nabla \cdot \boldsymbol{\mu} \rangle_c^{n+1/4} - \langle \nabla \cdot \boldsymbol{\mu} \rangle_c^{n-1/4})$$
$$- \Delta t^{n+1/2} \sum_{d \in \mathcal{D}(c)} (\sigma_{cd}^{n+1/2} \mathbf{s}_{cd}^{n+1/2} \cdot \mathbf{u}_c^{n+1/2} \rho_c^{n+1} e_c^{n+1/2} - \sigma_{dc}^{n+1/2} \mathbf{s}_{dc}^{n+1/2} \cdot \mathbf{u}_d^{n+1/2} \rho_d^{n+1} e_d^{n+1/2})$$
$$- \tfrac{1}{2}\Delta t^{n+1/2} \sum_{d \in \mathcal{D}(c)} \sigma_{cd}^{n+1/2} \mathbf{s}_{cd}^{n+1/2} \cdot \mathbf{u}_c^{n+1/2} \rho_c^{n+1} ((\boldsymbol{\mu}_d^{n+1/2})^2 - (\boldsymbol{\mu}_c^{n+1/2})^2)$$
$$+ \tfrac{1}{2}\Delta t^{n-1/2} \sum_{d \in \mathcal{D}(c)} \sigma_{cd}^{n-1/2} \mathbf{s}_{cd}^{n-1/2} \cdot \mathbf{u}_c^{n-1/2} \rho_c^n (\boldsymbol{\mu}_d^{n-1/2} - \boldsymbol{\mu}_c^{n-1/2}).(\boldsymbol{\mu}_d^{n+1/2} + \boldsymbol{\mu}_d^{n-1/2}) \qquad (9)$$

with

$$e_c^{n+1/2} = e_c^{n+1} + \tfrac{1}{2} \frac{\Delta t^{n+1/2}}{V_c^{n+1} \rho_c^{n+1}} [P+Q]_c^{n+1} \langle \nabla \cdot \boldsymbol{\mu} \rangle_c^{n+3/4} \, ,$$

$$\langle \nabla \cdot \boldsymbol{\mu} \rangle_c^{n \pm 1/4} = \sum_{d \in \mathcal{D}(c)} \left(\tfrac{1}{2}(1 + \sigma_{cd}^{n-1/2} - \sigma_{dc}^{n-1/2}) \mathbf{s}_{cd}^{n-1/2} \cdot \boldsymbol{\mu}_c^{n \pm 1/2} + \tfrac{1}{2}(1 - \sigma_{cd}^{n-1/2} + \sigma_{dc}^{n-1/2}) \mathbf{s}_{cd}^{n-1/2} \cdot \boldsymbol{\mu}_d^{n \pm 1/2} \right) .$$

Explicit numerical scheme eSMASH

Solving a linearly implicit system for iSMASH with a total number of cells I involves

- 1D : tridiagonal decomposition (algorithmic complexity $\mathcal{O}(3I)$)
- 2D : band matrix decomposition (algorithmic complexity $\mathcal{O}(I\sqrt{I})$)

For performance purposes, we propose an explicit version of iSMASH scheme

- Same discrete action integral than iSMASH
- Approximation of an explicit mass transport once variational equations are obtained (numerical residue of this approximation is at the scheme's order)
- eSMASH numerical scheme obtained by using the same global strategy of derivation as iSMASH

1) Explicit evolution of absolute velocity

$$V_c^n \rho_c^n (\boldsymbol{\mu}_c^{n+1/2} - \boldsymbol{\mu}_c^{n-1/2}) = -\Delta t^n \sum_{d \in \mathcal{D}(c)} \tfrac{1}{2}(1 + \sigma_{cd}^{n-1/2} - \sigma_{dc}^{n-1/2}) \mathbf{s}_{cd}^{n-1/2} (P_d^n - P_c^n)$$
$$+ \Delta t^{n-1/2} \sum_{d \in \mathcal{D}(c)} \sigma_{dc}^{n-1/2} \mathbf{s}_{dc}^{n-1/2} \cdot \mathbf{u}_d^{n-1/2} \rho_d^{n-1} (\boldsymbol{\mu}_d^{n-1/2} - \boldsymbol{\mu}_c^{n-1/2}) \,. \quad (10)$$

2) Choice of a grid velocity $\mathbf{w}_p^{n+1/2}$

3) Explicit evolution of mass transport

$$V_c^{n+1} \rho_c^{n+1} - V_c^n \rho_c^n = \Delta t^{n+1/2} \sum_{d \in \mathcal{D}(c)} (\sigma_{dc}^{n+1/2} \mathbf{s}_{dc}^{n+1/2} \cdot \mathbf{u}_d^{n+1/2} \rho_d^n - \sigma_{cd}^{n+1/2} \mathbf{s}_{cd}^{n+1/2} \cdot \mathbf{u}_c^{n+1/2} \rho_c^n) \quad (11)$$

4) Explicit evolution of internal energy

$$V_c^{n+1} \rho_c^{n+1} e_c^{n+1} - V_c^n \rho_c^n e_c^{n+1/2} = -\tfrac{1}{2} \Delta t^{n+1/2} [P+Q]_c^{n+1} \langle \nabla \cdot \boldsymbol{\mu} \rangle_c^{n+3/4}$$
$$- \frac{(\Delta t^{n+1/2} - \Delta t^{n-1/2})}{4} [P+Q]_c^n (\langle \nabla \cdot \boldsymbol{\mu} \rangle_c^{n+1/4} - \langle \nabla \cdot \boldsymbol{\mu} \rangle_c^{n-1/4})$$
$$- \Delta t^{n+1/2} \sum_{d \in \mathcal{D}(c)} (\sigma_{cd}^{n+1/2} \mathbf{s}_{cd}^{n+1/2} \cdot \mathbf{u}_c^{n+1/2} \rho_c^n e_c^{n+1/2} - \sigma_{dc}^{n+1/2} \mathbf{s}_{dc}^{n+1/2} \cdot \mathbf{u}_d^{n+1/2} \rho_d^n e_d^{n+1/2})$$
$$- \tfrac{1}{2} \Delta t^{n+1/2} \sum_{d \in \mathcal{D}(c)} \sigma_{cd}^{n+1/2} \mathbf{s}_{cd}^{n+1/2} \cdot \mathbf{u}_c^{n+1/2} \rho_c^n ((\boldsymbol{\mu}_d^{n+1/2})^2 - (\boldsymbol{\mu}_c^{n+1/2})^2)$$
$$+ \tfrac{1}{2} \Delta t^{n-1/2} \sum_{d \in \mathcal{D}(c)} \sigma_{cd}^{n-1/2} \mathbf{s}_{cd}^{n-1/2} \cdot \mathbf{u}_c^{n-1/2} \rho_c^{n-1} (\boldsymbol{\mu}_d^{n-1/2} - \boldsymbol{\mu}_c^{n-1/2}).(\boldsymbol{\mu}_d^{n+1/2} + \boldsymbol{\mu}_d^{n-1/2}) \quad (12)$$

with

$$e_c^{n+1/2} = e_c^n - \tfrac{1}{2} \frac{\Delta t^{n+1/2}}{V_c^n \rho_c^n} [P+Q]_c^n \langle \nabla \cdot \boldsymbol{\mu} \rangle_c^{n+1/4} \,,$$

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Numerical tests

Behavior of numerical schemes analyzed by performing several usual test cases involving shocks and advections (Sod, Sedov and Triple point tests)

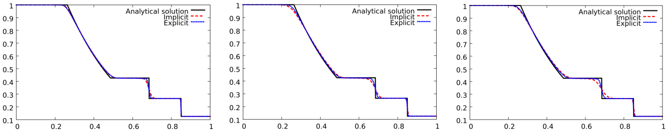
- In 1D for indifference to implicit (iSMASH) or explicit (eSMASH) advection
- In 2D for indifference to grid motion strategy (only eSMASH scheme)
- In 2D for versatility in the choice of grid velocity (only eSMASH)

In all test case results

- Fluid supposed to be a perfect gas $P = (\gamma - 1)\rho e$ with γ the isentropic coefficient
- Test results are moslty density profiles (velocity and pressure strongly correlated to density)
- Optimal values of artificial viscosity $P \longrightarrow P + Q$ where $a_1 = 0.5$ and $a_2 = \frac{\gamma+1}{2}$ [Lew, 2003]
- Time step of simulation bounded by usual CFL condition (sound velocity and advection)

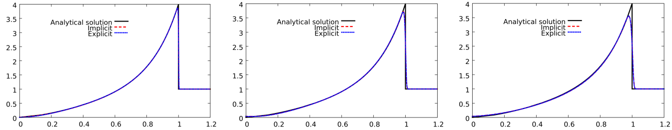
1D tests to indifference to implicit vs explicit advection

Sod's shock tube :
Left : $w = 0$
Center : $w = 2.2$
Right : $w = -1.2$



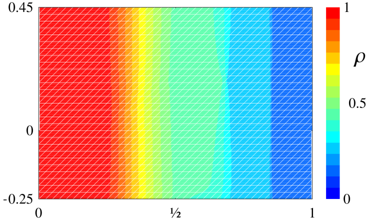
$I = 1000$ cells, $\mathrm{CFL} = 0.8$ for both implicit and explicit advections

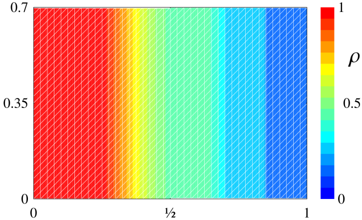
Plane Sedov's blast wave :
Left : $w = 0$
Center : $w = 1.2$
Right : $w = -1.2$

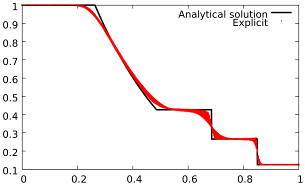


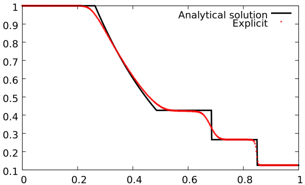
$I = 1000$ cells, $\mathrm{CFL} = 0.9$ for both implicit and explicit advections

2D tests to indifference to grid motion strategy



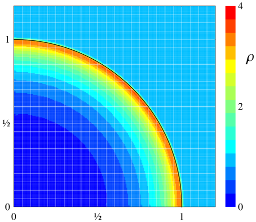


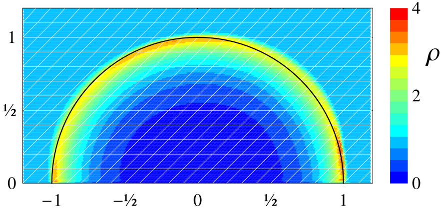


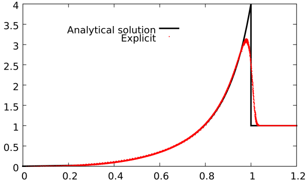


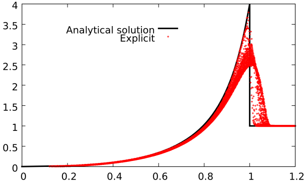
l	400x280	400x280
w	$w_x = 5y,\ w_y = 0$	$w_x = 0,\ w_y = 5x - 2.5$

2D tests to indifference to grid motion strategy





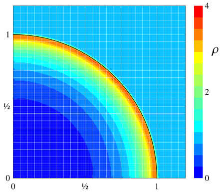


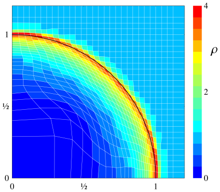


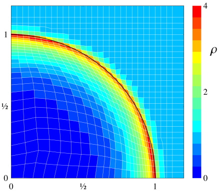
l	240x240	200x100
$\mathbf{w}$	$w_x = w_y = 0$	$w_x = y,\ w_y = 0$

2D illustrations of versatility in grid motion strategy

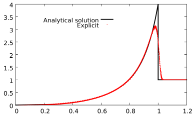
2D Sedov

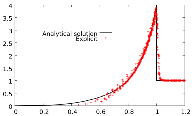


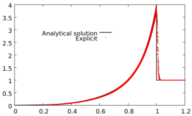




Density

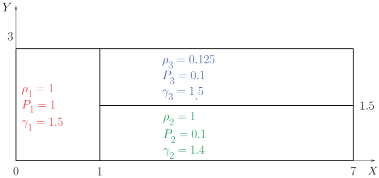


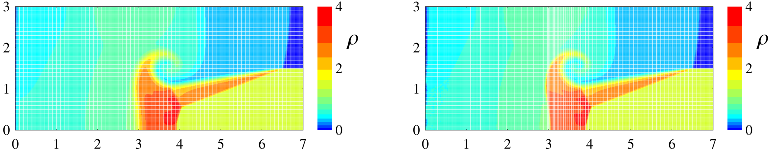




l	240x240	30x30	30x30
w	0	$0{,}99\boldsymbol{\mu}^{\mathrm{Lag}}$	$\tau\boldsymbol{\mu}^{\mathrm{Lag}}$ with $\tau = {(t/t_0)^2}/{1+(t/t_0)^2}$

Initial conditions of Triple point test





I	700x300	700x300
w	0	$<\mu_x^{\mathrm{Lag}}>_{y\in[0,1.5]}$

Outline

- Scientific context : ALE schemes and numerial mimetism
- Discrete derivation of the scheme
  - Discretization of fields and transport
  - Discrete action integral and Euler–Lagrange equations
  - Global strategy of derivation
  - Main steps of scheme
- Numerical tests
  - 1D indifference to implicit–explicit advection
  - 2D indifference to grid motion strategy
  - 1D–2D versatility in the choice of grid velocity
- Conclusions and perspectives

Conclusions and perspectives

In this work, presentation of a novel 2D scheme for simulating single-fluid compressible flows :

- Direct ALE formalism $\longrightarrow$ arbitrary evolution of grid
- Mimetic approach $\longrightarrow$ capture of pressure work thermodynamically consistent
- Exact conservation of mass, momentum and total energy
- Robustness and stability in presence of shocks and deformations

Perspectives and current works :

- To be submitted soon
- Second-order accuracy
- Extension to multiple fluids ($N > 2$)
- Exchange terms for gas–particles flows