A 3D Finite Volume Lagrangian Scheme

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Introduction

- **Lagrangian fluid dynamics is critical for ICF:**
  - **Strong** compressions,
  - Multi-material: avoid mixing.
  
  see P.H. MAIRE tomorrow

  R. ABGRALL, J. BREIL, P.H. MAIRE, and J. OVADIA. *A Lagrangian scheme for multidimensional compressible flow problems*. JCP, 2004. proposed alternatively to split \( p_r \) on each half-edge of each cell.

- Ongoing research about a new family of 3D Finite Volume schemes.

- In 2D this is based on B. DESPRÉS and C. MAZERAN. *Lagrangian Gas Dynamics in 2D and Lagrangian Schemes*, Arma 2005. PhD thesis to be defended soon.

- Finite Volume collocated schemes have a great potential for **ALE** developments and **remeshing** techniques since

  \[
  \rho, \mathbf{u} \text{ and } e = \varepsilon + \frac{1}{2} |\mathbf{u}|^2
  \]

  are discretized at the same place.
Euler equations in Lagrangian coordinates

\[
\begin{align*}
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) &= 0, \\
\frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla \cdot ((\rho \mathbf{u}) \mathbf{u}) + \nabla p &= 0, \\
\frac{\partial (\rho e)}{\partial t} + \nabla \cdot (e \mathbf{u}) + \nabla \cdot (p \mathbf{u}) &= 0.
\end{align*}
\]

Here we choose \( p = (\gamma - 1) \frac{e}{\rho} \)

Euler equations in Eulerian coordinates

\[
\begin{align*}
\rho \frac{d \mathbf{u}}{dt} - \nabla \cdot \mathbf{u} &= 0, \\
\rho \frac{d \mathbf{u}}{dt} + \nabla p &= 0, \\
\rho \frac{d e}{dt} + \nabla \cdot (e \mathbf{u}) &= 0,
\end{align*}
\]

where \( \tau = \frac{1}{\rho} \).
Construction of the scheme in 3D
Introducing $C_{jr}$

We construct a 3D scheme such that the density $\rho_j^n$, the velocity $u_j^n$ and the total energy $e_j^n$ are the unknowns given in cell $j$.

One can construct the vectors $C_{jr} \in \mathbb{R}^3$

$$C_{jr} = |C_{jr}| n_{jr}, \quad |C_{jr}| \approx area, \quad |n_{jr}| = 1.$$  

such that the volume of cell $j$ is

$$V_j = \frac{1}{3} \sum_r (C_{jr}, x_r)$$

and the derivative of the volume is

$$V_j'(t) = \sum_r (C_{jr}, u_r), \quad u_r(t) = x_r'(t).$$

For tetrahedra $C_{jr}$ are uniquely defined.  
For other cell types $C_{jr}$ are not uniquely defined.
Define the mass of the lagrangian cell

\[ M_j = \rho_j(t)V_j(t). \]

One has

\[ M_j \frac{d}{dt} \left( \frac{1}{\rho_j(t)} \right) = V_j'(t) = \sum_r (C_{jr}, u_r). \]

Therefore

\[ \sum_r (C_{jr}, u_r) \approx \int_{\partial_j} (u, n) d\sigma = \int_j \nabla \cdot u \, dx \]

is our Finite Volume discretization of the divergence operator.

⇒ The \( C_{jr} \)'s give the discretization of the divergence operator.
Discretization of the gradient

We use the idea of a **compatible discretization** of all discrete operators. One has the formula

\[ \sum_r C_{jr} p_r \approx \int_{\partial j} n_p \, d\sigma \quad \left( = \int_j \nabla p \, dx \right). \]

We have also

\[ \sum_r (C_{jr}, u_r) p_r \approx \int_{\partial j} (u, n) p \, d\sigma = \int_{\partial j} (u, p n) \, d\sigma \quad \left( = \int_j \nabla \cdot (p u) \, dx \right). \]

This gives the structure of the Finite Volume Lagrangian scheme

\[
\begin{cases}
V_j'(t) = \sum_r (C_{jr}, u_r), \\
M_j u'_j(t) = - \sum_r C_{jr} p_r, \\
M_j e'_j(t) = - \sum_r (C_{jr}, u_r) p_r.
\end{cases}
\]
Construction of the fluxes

At this stage we know only the unknowns inside the cells, that is $\rho_j(t)$, $u_j(t)$ and $e_j(t)$. So we need a formula to construct the $u_r$’s and $p_r$’s. We use mainly three ideas.

- The $p_r$ are replaced by some $p_{jr}$’s.
Construction of the fluxes

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- The $p_r$ are replaced by some $p_{jr}$’s.
- We assume the Riemann-invariant-like formula along $n_{jr}$

$$p_{jr} - p_j + \rho_j c_j (u_r - u_j, n_{jr}) = 0.$$
At this stage we know only the unknowns inside the cells, that is \( \rho_j(t), \mathbf{u}_j(t) \) and \( e_j(t) \). So we need a formula to construct the \( \mathbf{u}_r \)'s and \( p_r \)'s. We use mainly three ideas.

- The \( p_r \) are replaced by some \( p_{jr} \)'s.
- We assume the Riemann-invariant-like formula along \( \mathbf{n}_{jr} \)

\[
p_{jr} - p_j + \rho_j c_j (\mathbf{u}_r - \mathbf{u}_j, \mathbf{n}_{jr}) = 0.
\]

- We force the local conservativity of forces around node \( r \)

\[
\sum_j C_{jr} p_{jr} = \sum_j |C_{jr}| \mathbf{n}_{jr} p_{jr} = 0.
\]

There is a unique solution to these requirements.
Solution

After elimination of the $p_{jr}$'s, the equation for $u_r$ is

$$
\left( \sum_j \rho_j c_j |C_{jr}| n_{jr} \otimes n_{jr} \right) u_r
$$

$$
= \left( \sum_j C_{jr} p_j \right) + \left( \sum_j \rho_j c_j |C_{jr}| n_{jr} \otimes n_{jr} u_j \right).
$$

Since the matrix is symmetric and positive

$$
A_r = \left( \sum_j \rho_j c_j |C_{jr}| n_{jr} \otimes n_{jr} \right) = A_r^t > 0
$$

there is a unique solution $u_r$. Then we compute the $p_{jr}$'s thanks to

$$
p_{jr} - p_j + \rho_j c_j (u_r - u_j, n_{jr}) = 0.
$$
Scheme in 3D

- Cell quantities \((M_j, V_j, x_j, \rho_j, e_j, u_j \text{ and } p_j)\) are given
- Compute \(C_{jr}\) on the current configuration
- We take \(\Delta t \leq \min_j \left( \frac{\sum_r |C_{jr}|}{3V_j} c_j \right) \).
- \(A_r = \sum_j \rho_j c_j C_{jr} \otimes n_{jr}\).  
- \(u_r = A_r^{-1} \sum_j (C_{jr} p_j + \rho_j c_j C_{jr} \otimes n_{jr} u_j)\).
- \(p_{jr} = p_j + \rho_j c_j (u_j - u_r, n_{jr})\)
- \(u_{j}^{n+1} = u_j^n - \frac{\Delta t}{M_j} \sum_r C_{jr} p_r\)
- \(e_{j}^{n+1} = e_j^n - \frac{\Delta t}{M_j} \sum_r (C_{jr}, u_r) p_r\)
- \(x_{r}^{n+1} = x_r^n + \Delta t u_r\)
- Update \(V_j, \rho_j\) and \(p_j\)
Conservativity

- **Mass conservation:** the scheme imposes $M_j$ to be constant.
- **Momentum conservation:**
  \[
  \sum_j M_j u_j^{n+1} = \sum_j M_j u_j^n - \sum_j \Delta t \sum_r C_{jr} p_r \\
  = \sum_j M_j u_j^n - \Delta t \sum_r \sum_j C_{jr} p_r \\
  = \sum_j M_j u_j^n
  \]

- **Total energy conservation:**
  \[
  \sum_j M_j e_j^{n+1} = \sum_j M_j e_j^n - \sum_j \Delta t \sum_r \left( C_{jr}, u_r \right) p_r \\
  = \sum_j M_j e_j^n - \Delta t \sum_r \left( \sum_j C_{jr} p_r, u_r \right) \\
  = \sum_j M_j e_j^n
  \]

$\implies$ the scheme is **locally** conservative.

It is also stable and consistent.
Second order extension

• **Goal**
  - Improve the accuracy of the scheme.
  - Diminish scheme dissipation

• **Method. Muscl reconstruction + Van-Leer slope limiter:**
  
  • \( \tilde{u}_j(x) = u_j + \Phi^{vl} \nabla u_j(x - x_j) \)
  
  • \( \tilde{p}_j(x) = p_j + \Phi^{vl} \nabla p_j \cdot (x - x_j) \)

  \( \Phi^{vl} \in [0, 1] \) is chosen so that \( \tilde{p}_j \) and \( |\tilde{u}_j| \) respect some maximum principle.

Second order fluxes are

- \( u_r = A_r^{-1} \sum_j (C_{jr} \tilde{p}_j(x_r) + \rho_j c_j C_{jr} \otimes n_{jr} \tilde{u}_j(x_r)) \)

- \( p_{jr} = \tilde{p}_j(x_r) + \rho_j c_j (\tilde{u}_j(x_r) - u_r, n_{jr}) \)

The scheme is order 1 in time, so we need smaller time steps to avoid the anti-dissipative term of the equivalent equation.
Second order extension

- Second Method. Muscl reconstruction + LW procedure + Van-Leer slope limiter:
  
  \[ \bar{u}_j(x) = u_j + \Phi^{vl}(1 - \nu) \nabla u_j(x - x_j) \]
  
  \[ \bar{p}_j(x) = p_j + \Phi^{vl}(1 - \nu) \nabla p_j \cdot (x - x_j) \]

  \( \Phi^{vl} \in [0, 1] \) is chosen so that \( \bar{p}_j \) and \( |\bar{u}_j| \) respect some maximum principle.

Second order fluxes are still

- \( u_r = A_r^{-1} \sum_j \left( C_{jr} \bar{p}_j(x_r) + \rho_j c_j \ C_{jr} \otimes n_{jr} \ \bar{u}_j(x_r) \right) \).

- \( p_{jr} = \bar{p}_j(x_r) + \rho_j c_j \ (\bar{u}_j(x_r) - u_r, n_{jr}) \)

The scheme is formally order 2 in time and space for simple 1D problems.
Numerical results
Numerical results

We compute the results of some basic shock tube problems in various geometries.

**Sod shock tube**

\[ \gamma = 1.4, \quad u = 0 \]

\[ \begin{cases} 
  p(x) = 1 & \rho(x) = 1 \\
  p(x) = 0.1 & \rho(x) = 0.125 
\end{cases} \quad \text{if } x < 0.5, \\
\text{else.} \]

**Shestakov shock tube**

\[ \gamma = \frac{5}{3}, \quad u = 0 \]

\[ p = \frac{2}{3} \times 10^{14} \quad x_{\min}(0) = 0 \quad x_{\max}(0) = 0.75 \]

\[ u(x_{\max}(t)) = 2.5 \times 10^{7} \]

\[ u(x_{\min}(t)) = \begin{cases} 
  10^{8} \left( (1 - 10^{8}t)^{-0.25} - 1 \right), & \text{if } 0 \leq t < 0.9 \times 10^{-8}, \\
  10^{8}(10^{0.25} - 1) \approx 7.8 \times 10^{7}, & \text{if } 0.9 \times 10^{-8} \leq t < 10^{-8}, \\
  0 & \text{else.} 
\end{cases} \]

**Sod shock tube in 2D and 3D**

\[ \gamma = 1.4, \quad u = 0 \]

\[ \begin{cases} 
  p(r) = 1 & \rho(r) = 1 \\
  p(r) = 0.1 & \rho(r) = 0.125 
\end{cases} \quad \text{if } x > 0.5, \\
\text{else.} \]
Sod shock tube - 1D

Density 100 cells, $t = 0.2s$
Shestakov shock tube - 1D

Density 100 cells, \( t = 10.4 \times 10^{-9} \text{s} \)
Sod shock tube - 2D

Density  $100 \times 50$ cells, $t = 0.2s$
Sod shock tube - 2D

Density

$100 \times 50$ cells, $t = 0.2s$
Sod shock tube - 3D

Density 187,500 and 21,600 cells, $t = 0.2s$ (Parallel computation)
Sod shock tube - 3D

Density 187 500 and 21 600 cells, $t = 0.2s$ (Parallel computation)
Fix-up and optimizations
Hourglass with Noh

This has already been identified in 2D.

Noh problem in 2D: \( \gamma = \frac{5}{3}, \ \rho = 1, \ p = 0(\approx 10^{-6}), \ u = -e_r. \)

Using a polar mesh, one obtains
A fix-up

- $c_j \ll 1 \implies A_r$ nearly singular.

- Noh: $c_j \approx 10^{-3} \implies A_r = \sum_j \rho_j c_j \mathbf{C}_{jr} \otimes \mathbf{n}_{jr} \approx 0.

  \[ u_r = A_r^{-1} \sum_j (\mathbf{C}_{jr} \bar{p}_j(x_r) + \rho_j c_j \mathbf{C}_{jr} \otimes \mathbf{n}_{jr} \bar{u}_j(x_r)). \]

- Idea: increase $c$ when it is too small for the fluxes calculus (more dissipative scheme).
In order to increase the time step, we can replace

\[ p_{jr} - p_j + \rho_j c_j (u_r - u_j, n_{jr}) = 0 \]

by

\[ p_{jr} - p_j + \lambda_j \rho_j c_j (u_r - u_j, n_{jr}) = 0. \]

It can be shown that the optimal \( \lambda_j \) is

\[ \lambda_j = \sum_r \frac{|C_{jr}|}{\Lambda} \in [1, \sqrt{3}], \]

where \( \Lambda \) is the maximum eigenvalue of

\[ \sum_r \frac{C_{jr} \otimes C_{jr}}{|C_{jr}|}. \]

Finally \( \Delta t \leq \min_j \left( \lambda_j \frac{\sum_r |C_{jr}|}{3V_j c_j} \right) \)
Conclusions et perspectives

- The whole scheme relies on the definition of $C_{jr}$.
  - This is straightforward only for tetrahedrons.
  - But there is no unique definition for other kind of meshes in 3D. So we need to compare all possible definition of these quantities.
  - The situation is different in 2D (unicity of the definition for all meshes).
- We still work on boundary conditions and the second order Muscl reconstruction.
- We have begun the evaluation of the coupling with ALE and remeshing.
- We shall start coupling with other physics to test this scheme for ICF simulations.
- ...