A cell-centered Arbitrary Lagrangian Eulerian method for two-dimensional multimaterial problems

Application to Inertial Confinement Fusion modeling in the direct drive context

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Introduction and motivations

- ICF plasma is created by laser interaction with target
- ICF target is the assembly of multimaterial layers with high aspect ratios
- Multimaterial flows with large displacements, strong shocks and rarefaction waves
- Simulations with large changes of computational domain volume and shape (animation)
- Lagrangian formulation is well adapted to ICF flows
  - Mesh moves with the fluid
  - Shock resolution is increased
  - No mass flux between cell
  - Free surfaces are naturally treated
  - Interfaces are sharply resolved
- However for too large deformations (shear and vorticity) it appears a lack of robustness (mesh tangling)
- It can be treated by using an Arbitrary Lagrangian Eulerian (ALE) strategy
ALE strategy

- Lagrangian phase
  - New second order cell-centered Lagrangian scheme*
  - Conservative and entropy consistent
  - Cell-centered momentum easier to handle in view of ALE

- Rezoning phase
  - Improvement of geometric quality of the grid
  - Quasi Lagrangian interface tracking using Bezier curves

- Remapping phase
  - Conservative transfer from the Lagrangian mesh to the rezoned
  - Swept displacement face flux computation
  - Second order accuracy

Governing equations

**ALE form of the compressible Euler equations**

For a moving control volume $\Omega(t)$ whose boundary’s velocity is $\dot{X}$

$$\frac{d}{dt} \int_{\Omega(t)} d\Omega - \int_{\partial\Omega(t)} \dot{X} \cdot N \, dl = 0,$$

**geometric conservation law**

$$\frac{d}{dt} \int_{\Omega(t)} \rho d\Omega + \int_{\partial\Omega(t)} \rho \left( \mathbf{V} - \dot{X} \right) \cdot N \rho \, dl = 0,$$

$$\frac{d}{dt} \int_{\Omega(t)} \rho \mathbf{V} d\Omega + \int_{\partial\Omega(t)} \left[ \left( \mathbf{V} - \dot{X} \right) \cdot N \rho \mathbf{V} + P N \right] \, dl = 0,$$

$$\frac{d}{dt} \int_{\Omega(t)} \rho E d\Omega + \int_{\partial\Omega(t)} \left[ \left( \mathbf{V} - \dot{X} \right) \cdot N \rho E + P \mathbf{V} \cdot N \right] \, dl = 0.$$

**Equation of state:** $P \equiv P(\rho, \varepsilon)$ where $\varepsilon = E - \frac{1}{2} |\mathbf{V}|^2$.

For $\dot{X} = \mathbf{V}$ (resp. $\dot{X} = 0$) we recover the Lagrangian (resp. Eulerian) formulation.
Lagrangian phase

Evolution equations for the discrete unknowns \((\tau_c = \frac{1}{\rho_c}, V_c, E_c)\)

\[
m_c \frac{d}{dt} \tau_c - \sum_{n \in \mathcal{N}(c)} \left( L_n^c N_n^c + L_n^c N_n^c \right) \cdot V_n^* = 0,
\]

\[
m_c \frac{d}{dt} V_c + \sum_{n \in \mathcal{N}(c)} \left( L_n^c P_n^*,c N_n^c + L_n^c P_n^*,c N_n^c \right) = 0,
\]

\[
m_c \frac{d}{dt} E_c + \sum_{n \in \mathcal{N}(c)} \left( L_n^c P_n^*,c N_n^c + L_n^c P_n^*,c N_n^c \right) \cdot V_n^* = 0,
\]

where \(\mathcal{N}(c)\) is the set of vertices of cell \(c\).

Node motion

\[
\frac{d}{dt} X_n = V_n^*, \quad X_n(0) = x_n.
\]

Construction of a nodal solver to evaluate the nodal fluxes \(V_n^*, P_n^*, c\) and \(P_n^*, c\).
Lagrangian phase

Computation of the nodal fluxes $V^*_n$, $P^*_{n,c}$ and $P^*_{\overline{n},c}$

Let $M^c_n = Z_c \left( L^c_n N^c_{\overline{n}} \otimes N^c_n + L^c_n N^c_n \otimes N^c_{\overline{n}} \right)$

$$V^*_n = \left( \sum_{c \in C(n)} M^c_n \right)^{-1} \sum_{c \in C(n)} \left[ \left( L^c_n N^c_{\overline{n}} + L^c_n N^c_n \right) P_c + M^c_n V_c \right],$$

where $C(n)$ is the set of the cells sharing node $n$.

$$P_c - P^*_{n,c} = Z_c (V^*_n - V_c) \cdot N^c_{\overline{n}},$$

Riemann invariants

$$P_c - P^*_{\overline{n},c} = Z_c (V^*_n - V_c) \cdot N^c_{\overline{n}},$$

We can check that these fluxes lead to a conservative and entropy consistent scheme. For 1D flows, we recover exactly the Godunov acoustic fluxes.
Lagrangian phase

- Second order extension
  - Piecewise linear reconstruction $\phi_c(X) = \phi_c + \nabla \phi_c \cdot (X - X_c)$
  - Computation of $\nabla \phi_c$ by a least squares procedure
  - Reconstruction exact for linear fields
  - Monotony ensured by slope limiters so that

$$\min_{k \in \mathcal{C}(c)} \phi_k \leq \phi_c(X_n) \leq \max_{k \in \mathcal{C}(c)} \phi_k,$$

where $\mathcal{C}(c)$ is the set of the nearest neighbors of cell $c$.

- Extrapolated values of $P$ and $V$ at the nodes for the nodal solver
- Explicit time discretization by a 2 steps Runge-Kutta procedure
Numerical results

Sedov test case on a $50 \times 50$ Cartesian grid

Density map (left) and density in all the cells (right) at $t = 1$.

Numerical results

Sedov test case on a polygonal grid

Density map (left) and density in all the cells (right) at $t = 1$. 
Numerical results

Cylindrical Noh test case on a non-conformal grid

Initial mesh
Non-conformal mesh with 2 levels of refinement, 2250 cells mix of triangles, quadrangles and pentagons.

Zoom on the final mesh
Numerical results

Cylindrical Noh test case on a non-conformal grid

Density in all the cells at $t = 0.6$
Rezoning phase

- Unstructured mesh quality optimization
  - Construct local nodally based objective functions [Knupp (IJNME, 2000)]
  - Minimize separately each of the local objective function
  - Iterate over all the nodes of the mesh

- Treatment of boundary and interface nodes
  - Free boundaries and interfaces are fitted with Bezier curves
  - Nodes are assigned to move on these Bezier curves
  - It leads to constrained minimization problems

- Mesh untangling by combination of feasible set method and numerical optimization [Vachal, Garimella, Shashkov (JCP, 2004)].

- Main issue: keep the rezoned mesh as close to Lagrangian as possible by using relaxation criteria related to mesh quality measurements [Ph. Hoch (2007)]
Mesh optimization

Nodal objective function

Jacobian matrices related to \( c \) and \( N(x, y) \)

\[
\begin{align*}
J_c &= (NN_c, NN_m) \\
J_n &= (N_c N_p, N_c N) \\
J_m &= (N_m N, N_m N_l)
\end{align*}
\]

The displacement of \( N(x, y) \) is computed by minimizing

\[
F(x, y) = \sum_{c \in C(N)} \frac{\|J_c\|^2}{|\det J_c|} + \frac{\|J_n\|^2}{|\det J_n|} + \frac{\|J_m\|^2}{|\det J_m|}
\]

with a Newton procedure (single step towards the minimum). This objective function is closely related to the Winslow smoother.
Mesh optimization

Treatment of interface nodes

• \( N_i \)

Interpolated Bezier curve for \( t \in [0, 1] \)

\[
x(t) = (1 - t)^2 x_m + 2(1 - t)tx_i + t^2 x_p \\
y(t) = (1 - t)^2 y_m + 2(1 - t)ty_i + t^2 y_p
\]

Control point \( N_i \) is computed such that \( N_q \) is on the curve with parameter \( t_q = 0.5 \).

The displacement of \( N_q \) is computed by minimizing the objective function

\[
\Phi(t) = F[x(t), y(t)], \text{ with } t \in [0, 1] \]

Treatment of symmetry axis nodes

Symmetry axis is the straight line \( ax + by + c = 0 \), then the displacement of \( N_q \) is computed by minimizing the objective function \( F'(x, y) + \Lambda(ax + by + c) \) where \( \Lambda \) is a Lagrange multiplier.
Relaxation criterion

Nodality quality (cf. Ph. Hoch talk)

Quality based on angle or area

\[ Q_{\text{N}}^{\text{sin}} = \frac{\min_{c \in C(N)} \left[ \sin \alpha^c_m, \sin \alpha^c, \sin \alpha^c_n \right]}{\max_{c \in C(N)} \left[ \sin \alpha^c_m, \sin \alpha^c, \sin \alpha^c_n \right]} \]

\[ Q_{\text{N}}^{\text{area}} = \frac{\min_{c \in C(N)} \left[ A^c_m, A^c, A^c_n \right]}{\max_{c \in C(N)} \left[ A^c_m, A^c, A^c_n \right]} \]

For quadrangular grids with high aspect ratios we use \( Q_{\text{N}}^{\text{sin}} \) quality. The relaxed mesh is defined by

\[ X_{\text{N}}^{\text{rel}} = \omega_N X_{\text{N}}^{\text{rez}} + (1 - \omega_N) X_{\text{N}}^{\text{Lag}}, \text{ with } \omega_N = \min \left[ 1, \max \left( 0, \frac{Q_{\max} - Q_{\text{N}}^{\text{sin}}}{Q_{\max} - Q_{\min}} \right) \right] \]

where \( Q_{\max} = \sin \theta_{\max}, Q_{\min} = \sin \theta_{\min} \) with \( \theta_{\min} = 0 \) and \( \theta_{\max} = \pi/2 \).
Remapping phase

- Conservative interpolation of \((\rho, \rho V, \rho E)\) from the Lagrangian mesh to the new relaxed mesh
- Piecewise monotonic linear reconstruction over the Lagrangian mesh
- Remapping expressed in terms of fluxes across cell faces
- Approximate quadrature over regions swept by edges moving from Lagrangian position to the relaxed position
- Integral over new cells = sum of integrals over swept regions
- Cheaper than exact integration for which intersections is needed
Numerical results

Three materials instability

Shock wave interacting with a triple point

- Cartesian mesh $70 \times 30$ cells, $t_{\text{end}} = 5$
- Lagrange, ALE and Euler second order computations
- Concentration equations for ALE and Euler
- Mixture assumption isoP, isoT

\begin{align*}
\rho_1 &= 1 \\
P_1 &= 1 \\
\gamma_1 &= 1.5 \\
\rho_3 &= 0.125 \\
P_3 &= 0.1 \\
\gamma_3 &= 1.6 \\
\rho_2 &= 1 \\
P_2 &= 0.1 \\
\gamma_2 &= 1.4
\end{align*}
Numerical results

Three materials instability: Lagrangian computation

$C_2$ map at $t = 2.5$

Zoom on the vortex

Lagrangian computation fails due to the tangled mesh
Numerical results

Three materials instability: Lagrange and ALE at $t = 2.5$

We note the efficiency of the mesh relaxation based on angle criterion
Numerical results

Three materials instability: ALE and EULER at $t = 2.5$

We note the diffusion of the interface in the Eulerian case
Numerical results

- Non-linear phase of Richtmyer-Meshkov instability

Ref: C. Mügler, L. Hallo et al., Validation of an ALE Godunov Algorithm for Solutions of the Two-Species Navier-Stokes Equations, AIAA 96-2068, June 1996.

\[ \rho_1 = 1.206 \]
\[ \gamma_1 = 1.4 \]
\[ P_0 = 1.013 \times 10^5 \]
Air

\[ \rho_2 = 0.1663 \]
\[ \gamma_2 = 1.67 \]
\[ P_0 = 1.013 \times 10^5 \]
Helium

Transmitted shock
Reflected rarefaction wave
\[ a_0 = 0.32 \times 10^{-2} \]

- Initial perturbation \( X_{\text{inter}} = 0.4 + a_0 \cos \left( \frac{2\pi Y}{\lambda} \right) \)
- ALE second order calculation
- Mixture assumption isoP, isoT
- 3 Meshes, cell sizes: \( 2 \times 2 \) mm\(^2\), \( 1 \times 1 \) mm\(^2\) and \( 0.5 \times 0.5 \) mm\(^2\)
ALE results

X-t diagram of the flow
ALE results

Non-linear phase of Richtmyer-Meshkov instability

Cell size $2 \times 2 \ mm^2$

Cell size $1 \times 1 \ mm^2$

Cell size $0.5 \times 0.5 \ mm^2$

Concentration maps at $t = 15.973 \times 10^{-4} \ s$
Characterization of non local heat transport

- Plastic target with Vanadium and Titanium markers of 200 µm thickness
- Vanadium marker of 0.1 µm thickness at 5 µm
- Titanium marker of 0.1 µm thickness at 15 µm
- Include steady state radiative physics and transverse MHD
- LIL laser beam: \( \lambda = 0.35 \) µm, maximal intensity \( 1.10^{15} \) W cm\(^{-2}\)
- ALE computation with Bezier curves for interface and free boundary tracking

Experiment restitution

Map of ionization level and electron temperature
Conclusions and perspectives

- An accurate and robust 2D cell-centered unstructured second order ALE scheme
- Coupling with diffusion scheme (ICF code)
- Concentration equations with mixture assumptions
- Future works
  - Improvement of the mesh relaxation strategy
  - Coupling with interface reconstruction (cf. S. Galera’s talk)