Applications of ALE Method to Laser Plasma Studies

R. Liska¹, M. Kuchařík², J. Limpouch¹, P. Váchal¹

¹Czech Technical University in Prague, Czech Republic
liska@siduri.fjfi.cvut.cz
²Los Alamos National Laboratory, USA

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Overview

• motivation example for Lagrangian formulation

• hydrodynamical model with heat conductivity and laser absorption

• numerical methods used in our PALE (Prague ALE) code
  – hyperbolic part – Arbitrary Lagrangian Eulerian (ALE) method
  – parabolic part – heat conductivity
  – laser absorption – source term in internal energy equation

• laser plasma application, which cannot be treated by pure Lagrangian method
  – high velocity impact problem
  – double foil target
  – foam target
Motivation for Lagrangian Formulation

• laser plasma is created by laser interaction with targets

• target is \(0.8\mu m\) thin Aluminum foil; Prague Asterix Laser System (PALS) laser at 3-rd harmonics, pulse duration 250\(ps\), focus 40\(\mu m\), energy 200\(J\); animation

• computational mesh is fixed to the fluid and moves with the fluid

• no mass flux between cells through edges

• computation domain changes with time

• problems with large changes of computational domain volume and/or shape (compression or expansion)

• naturally treated moving boundaries

• typically used in laser plasma simulations
Euler Equations in Lagrangian Coordinates

- density \( \rho \), velocity \( \mathbf{u} \), pressure \( p \), internal energy \( \epsilon = E/\rho - \frac{u^2}{2} \),
- temperature \( T \), heat conductivity \( \kappa \), laser intensity \( I \)

\[
\begin{align*}
\frac{d\rho}{dt} + \rho \text{ div } \mathbf{u} &= 0, \\
\frac{d\mathbf{x}}{dt} &= \mathbf{u} \\
\rho \frac{d\mathbf{u}}{dt} + \text{ grad } p &= 0 \\
\rho \frac{d\epsilon}{dt} + p \text{ div } \mathbf{u} &= -\text{ div}(\mathbf{I}) + \text{ div}(\kappa \text{ grad } T)
\end{align*}
\]

- total Lagrangian time derivatives include convective terms

\[
\frac{d}{dt} = \frac{\partial}{\partial t} + \mathbf{u} \cdot \text{ grad}
\]

- equation of state – ideal gas and QEOS for plasma
- splitting – hyperbolic and parabolic part
- heat conductivity essential – faster shock wave
Moving Lagrangian Mesh

- moving mesh can degenerate

initial | Lagr | ALE

degenerate typically for shear flow like high velocity impact

can be treated by ALE method
ALE Method

- ALE – Arbitrary Lagrangian Eulerian method. Combination of Lagrangian and Eulerian methods [Hirt, Amsden, Cook (JCP 1974, 1997)]
  - I. Lagrangian computation several time steps
  - II. Rezoning – mesh untangling and smoothing
  - III. Remapping – conservative interpolation of the conservative quantities from old to new, better mesh. Then, back to Lagrangian computation.

- remapping corresponds to Eulerian part of ALE method, allows mass flux between cells

- ALE method combines positives of both approaches – grid moves with fluid (as Lagrangian), but Eulerian part keeps it smooth
I. Lagrangian Step

- staggered discretization – scalar quantities (density, pressure, internal energy, temperature) defined inside grid cells, vector quantities (positions, velocities) defined on grid nodes

- compatible method [Caramana, Burton, Shashkov, Whalen (JCP, 1998)]

- based on zonal, subzonal, and viscosity forces in each grid node

  - zonal pressure force – force from all neighboring grid cells to the node due to the pressure inside cells
  - subzonal pressure force – depends on difference between pressure in cell, and the pressure in cell corners, reduces artificial grid distortions
  - viscosity force – adds artificial viscosity in compression regions; edge [Caramana, Shashkov, Whalen (JCP, 1998)] or tensor [Campbell, Shashkov (2000)] viscosity
II. Rezoning

• rezoning – mesh untangling and smoothing.
• for remapping we need to move only those vertices which are necessary and as little as possible

• simple smoothing [Winslow (1963)]

\[
x^{k+1}_{i,j} = \frac{1}{2(\alpha^k + \gamma^k)} \left( \alpha^k (x^{k}_{i,j+1} + x^{k}_{i,j-1}) + \gamma^k (x^{k}_{i+1,j} + x^{k}_{i-1,j})
\right.

\left. - \frac{1}{2} \beta^k (x^{k}_{i+1,j+1} - x^{k}_{i-1,j+1} + x^{k}_{i-1,j-1} - x^{k}_{i+1,j-1}) \right),
\]

where coefficients \( \alpha^k = x_\xi^2 + y_\xi^2 \), \( \beta^k = x_\xi x_\eta + y_\xi y_\eta \), \( \gamma^k = x_\eta^2 + y_\eta^2 \), and where \((\xi, \eta)\) are logical coordinates.

• Reference Jacobian method [Knupp, Margolin, Shashkov (JCP, 2002)]

• combination of feasible set method and numerical optimization [Váchal, Garimella, Shashkov (JCP, 2004)].
III. Remapping/1

- conservative interpolation of conservative quantities from the old Lagrangian mesh to the new smoothed mesh

1. piecewise linear reconstruction with Barth-Jasperson limiter [Barth (1997)]

   \[ g(x, y) = g_c + \left( \frac{\partial g}{\partial x} \right)_c (x - x_c) + \left( \frac{\partial g}{\partial y} \right)_c (y - y_c) \]

2. quadrature of reconstruction over cells of new mesh
   - exact quadrature – intersection of new cell with all neighboring old cells

* old mesh dashed, new mesh solid

* integration of linear function over each intersection polygon – Green theorem transforms into integration over polygon edges
III. Remapping/2

– **approximate quadrature** over regions swept by edges moving from old to new position [Kuchařík, Shashkov, Wendroff (JCP, 2003)]

– exact integration is very expensive, requires finding intersections.

– integral over new cell can be decomposed as sum of integrals over swept regions.

3. repair

  – Barth-Jasperson limiter guarantees monotonicity in 1D
  – in 2D new local local extrema might appear – repair [Shashkov, Wendroff (JCP, 2004)]

  • remapping of staggered quantities more complicated
ALE in cylindrical geometry

- generalized to cylindrical $r, z$ geometry [Kuchařík, Liska, Loubere, Shashkov (HYP2006)]

- additional factor $r$ in integrals
  \[
  \int f(x, y) \, dx \, dy \to \int f(r, z) \, r \, dr \, dz
  \]

- Lagrangian step
  - control volume method
  - cell center moved to center of cell mass instead of original average of vertexes – so that ALE remapping can be conservative

- rezoning – mesh nodes move on the $z$ axis

- remapping – additional factor $r$ in integrals
Heat Conductivity

- heat conductivity represented as parabolic term in the energy equation. By splitting, we solve $aT_t + \text{div} w = 0$, $w = -\kappa \text{grad} T = 0$ using mimetic operators method [Shashkov, Steinberg (1996)]

- mimetic discrete operators $G, D$ have the same discrete integral properties, namely gradient is adjoint of divergence $G = D^*$

$$a\frac{T^{n+1} - T^n}{\Delta t} + DW^{n+1} = 0$$

- implicit scheme in flux form

$$W^{n+1} - GT^{n+1} = 0$$

- temperature $T^{n+1}$ is eliminated and the system is solved for heat flux $W^{n+1}$; the matrix of the system is symmetric and positive definite; same time step as in hyperbolic Lagrangian/ALE step

- computed fluxes have to be smaller than physical heat flux limit $W^{n+1} = \text{sign}W^{n+1} \min(|W^{n+1}|, W_{\text{limit}})$

- generalization to cylindrical geometry.
Laser absorption

- simplest model – laser penetrates till critical density $\rho_c$ and is absorbed on the critical surface

- source in internal energy equation $\rho \frac{d \epsilon}{dt} + p \text{div} \ u = -\text{div}(I)$

- ray tracing model – curved rays with refraction, no reflected wave [N. Demchenko]
High velocity impact

• disc flyer impact problem

• high power laser-irradiated Aluminum disc ablatively accelerates up to very high velocity (40-190 km/s) and strikes to massive Aluminum target

• $d = 6; 11 \mu m, r = 150 \mu m, L = 200 \mu m$, laser energy $120 - 390 J$, 1-st or 3-rd harmonics, pulse length 400 ps, focus $r_f = 125 \mu m$.

• problem split into two parts for simulations:
  – ablative disc flyer acceleration by laser beam; animation
  – impact of disc flyer into massive target

• problem parameters similar to the experiment performed on the PALS laser facility in Prague [Borodziuk et al. CJP (2003), Kálal et al. ECLIM (2004)].
Crater creation

- after impact – increase of temperature, metling and evaporating material, circular shock wave
- crater (gas - liquid interface) formed inside the target

- temperature animation

- simulated craters size and shape correspond reasonably well to experimental data [Kuchařík, Liska, Limpouch (2006)]
Double foil target

- foils thickness $d_u = 0.8\mu m$, $d_l = 2\mu m$
- foils distance $L = 360\mu m$
- laser energy 78 J, 3-rd harmonics, pulse length 250 ps, focus $r_f = 40\mu m$
- almost vacuum between foils
- mass of neighboring vacuum and foils cells should not differ much
- vacuum cells are big while foils cells small
- initially e.g. one foil rectangular cell has $r/z$ edges lengths ratio $10^4$ and neighbors the vacuum cell with $r/z$ ratio 0.2
- pure Lagrangian simulation fails due to mesh degeneration soon after laser burns through the upper foil
Double foil target – ALE results

- laser maximum is at 0 ps

\[ \rho \left[ \text{g/cm}^3 \right] \text{ at 0 ps} \quad \rho \left[ \text{g/cm}^3 \right] \text{ at 100 ps} \quad p \left[ \text{g/(s}^2\text{cm)} \right] \text{ at 100 ps} \quad T \left[ \text{eV} \right] \text{ at 100 ps} \]

- double foil target density and pressure animation
Foam target

- 400 μm thick TAC foam with density 9.1 mg/cm$^3$ with 2 μm pores.

- Gaussian laser pulse on the third harmonics with wavelength 0.438 μm, total energy 170 J, the radius of laser spot on target 300 μm and FWHM length 320 ps.

- foam modelled by uniform density 9.1 mg/cm$^3$ material

Evolution of temperature; timing relates to the laser pulse maximum at 0 ps.
**Foam target - structured model**

- foam modelled by the sequence of $d_s = 0.018 \mu m$ thick dense slabs with density $\rho_s = 1 \text{ g/cm}^3$ separated by $d_v = 1.982 \mu m$ thick voids with density $\rho_v = 1 \text{ mg/cm}^3$

- experimental speed of laser penetration into the foam is about $600 \sim 700 \mu m/\text{ns}$, speed from structured simulation is about $500 \mu m/\text{ns}$ (average in time interval $(0.1, 0.5) \text{ ns}$) and from uniform simulation about $1600 \mu m/\text{ns}$ (average in time interval $(0.0, 0.25) \text{ ns}$).

- structured model approximates experimental data much better.
Foam target - structured model/2

- evolution of density and temperature

-200 ps

-100 ps

0 ps

\[ \rho \text{[g/cm}^3\text{]} \]

-200 ps

-100 ps

0 ps

\[ T \text{[eV]} \]

- density animation, zoomed animation,
Conclusion

- ALE method in Cartesian and cylindrical geometry
- heat conductivity, laser absorption
- applications – simulations of disc flyer, double foil and foam targets from PALS experiments
- pure Lagrangian simulation fails while ALE gives reasonable results
- perspectives – multimaterial, two temperature model, radiation transport, AMR........