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

Thanks to M. Shashkov, B. Wendroff, R. Loubère, N. Demchenko

Multimat Prague

September 14, 2007

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 250ps, focus $40\mu m$, energy 200J; 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)
- naturaly treated moving boundaries
- typically used in laser plasma simulations

Euler Equations in Lagrangian Coordinates

• density ρ , velocity \mathbf{u} , pressure p, internal energy $\epsilon = E/\rho - \mathbf{u}^2/2$, temperature T, heat conductivity κ , laser intensity I

$$\frac{d \rho}{d t} + \rho \operatorname{div} \mathbf{u} = 0, \qquad \frac{d \mathbf{x}}{d t} = \mathbf{u}$$

$$\rho \frac{d \mathbf{u}}{d t} + \operatorname{\mathbf{grad}} p = 0$$

$$\rho \frac{d \epsilon}{d t} + \rho \operatorname{div} \mathbf{u} = -\operatorname{div}(\mathbf{I}) + \operatorname{div}(\kappa \operatorname{\mathbf{grad}} T)$$

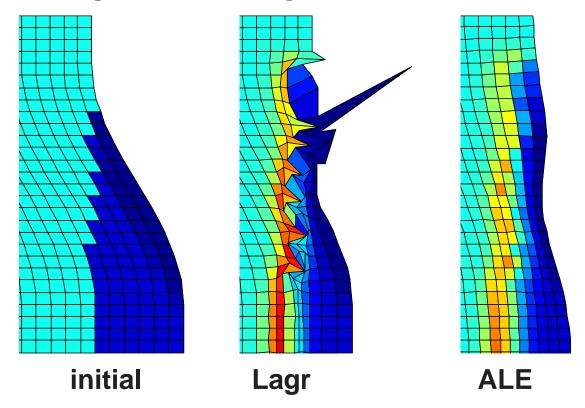
total Lagrangian time derivatives include convective terms

$$\frac{d}{dt} = \frac{\partial}{\partial t} + \mathbf{u} \cdot \mathbf{grad}$$

- 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



- degenerate typicaly 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)]
 - 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 smothing [Winslow (1963)]

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

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 (ξ,η) are logical coordinates.

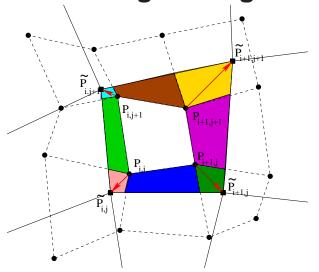
- Reference Jacobian method [Knupp, Margolin, Shashkov (JCP, 2002)]
- combination of feasible set method and numerical optimization [Váchal, Garimella, Shashkov (JCP, 2004)].

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

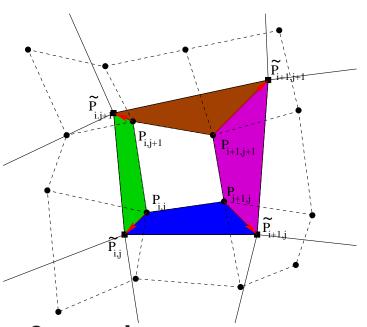


- * old mesh dashed, new mesh solid
- integration of linear function over each intersection polygon – Green theorem transforms into integration over polygon edges

III. Remapping/2

 approximate quadrature over regions swept by edges moving form 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 quarantees 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

$$\int f(x,y)dxdy \to \int f(r,z)rdrdz$$

- 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
- ullet rezoning mesh nodes move on the z axis
- ullet remapping additional factor r in integrals

Heat Conductivity

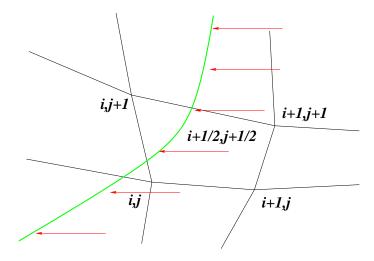
- heat conductivity represented as parabolic term in the energy equation. By splitting, we solve $aT_t + \text{div}\mathbf{w} = 0$, $\mathbf{w} = -\kappa \operatorname{\mathbf{grad}} T = 0$ using mimetic operators method [Shashkov, Steinberg (1996)]
- mimetic discrete operators G,D have the same discrete integral properties, namely gradient is adjoint of divergence $G=D^*$
- implicit scheme in flux form

$$a\frac{T^{n+1} - T^n}{\Delta t} + D\mathbf{W}^{n+1} = 0$$
$$\mathbf{W}^{n+1} - GT^{n+1} = 0$$

- temperature T^{n+1} is eliminated and the system is solved for heat flux \mathbf{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 $\mathbf{W}^{n+1} = \operatorname{sign} \mathbf{W}^{n+1} \min(|\mathbf{W}^{n+1}|, W_{limit})$
- generalization to cylindrical geometry.

Laser absorption

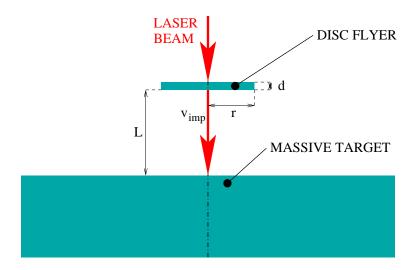
• simplest model – laser penetrates till critical density ρ_c and is absorbed on the critical surface



- source in internal energy equation $\rho \frac{d \epsilon}{d t} + p \operatorname{div} \mathbf{u} = -\operatorname{div}(\mathbf{I})$
- ray tracing model curved rays with refraction, no reflected wave [N. Demchenko]

High velocity impact

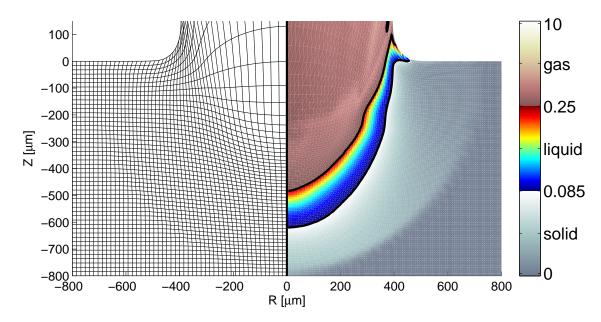
- disc flyer impact problem
- high power laser-irradiated Aluminum disc ablatively accelerates up to very high velocity (40-190 km/s) and strikes to massive Aluminum target
- $d=6;11\mu m, r=150\mu m, L=200\mu m$, laser energy $120-390\,\mathrm{J}$, 1-st or 3-rd harmonics, pulse length $400\,\mathrm{ps}$, focus $r_f=125\,\mu\mathrm{m}$.



- 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

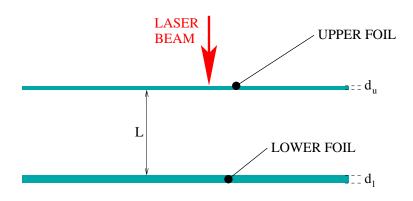
- after impact increase of temperature, metling and evaporating material, circular shock wave
- crater (gas liquid interface) formed inside the target



- temperature animation
- simulated craters size and shape correspond reasonably well to exparimental data [Kuchařík, Liska, Limpouch (2006)]

Double foil target

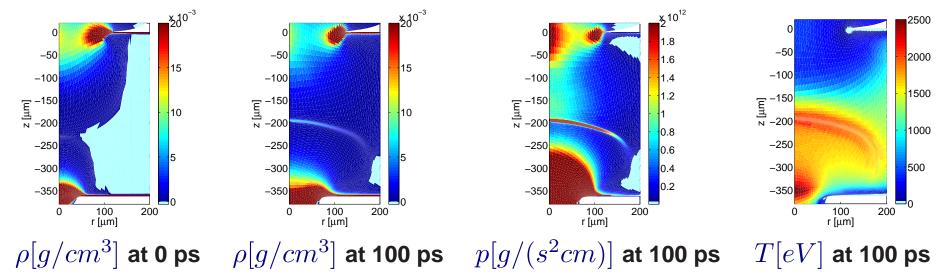
- foils thickness $d_u = 0.8 \mu m, d_l = 2 \mu m$
- foils distance $L=360\mu m$
- laser energy $78\,\mathrm{J}$, 3-rd harmonics, pulse length $250\,\mathrm{ps}$, focus $r_f = 40\,\mathrm{\mu m}$



- almost vaccum between foils
- mass of neighboring vaccum and foils cells should not differ much
- vaccum 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 vaccum 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

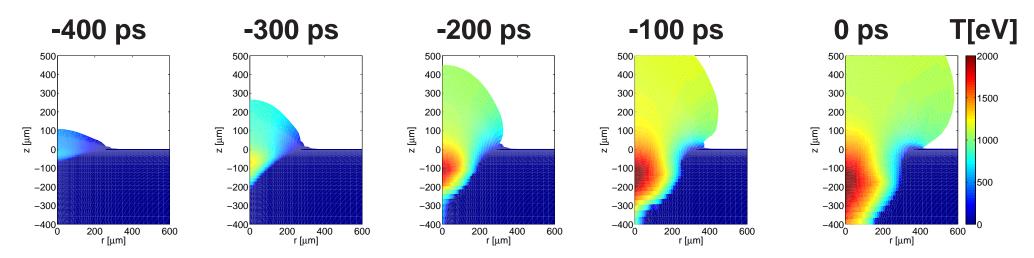
laser maximum is at 0 ps



double foil target density and pressure animation

Foam target

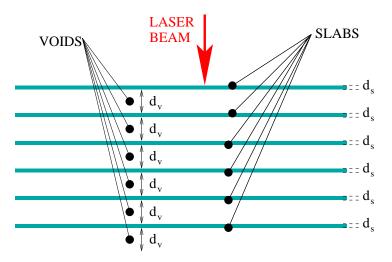
- $400 \mu \ \mathrm{m}$ thick TAC foam with density $9.1 \mathrm{mg/cm}^3$ with $2 \mu \mathrm{m}$ pores.
- Gaussian laser pulse on the third harmonics with wavelength $0.438\,\mu\mathrm{m}$, total energy $170\,\mathrm{J}$, the radius of laser spot on target $300\,\mu\mathrm{m}$ and FWHM length $320\,\mathrm{ps}$.
- ullet foam modelled by uniform density $9.1 \mathrm{mg/cm}^3$ material

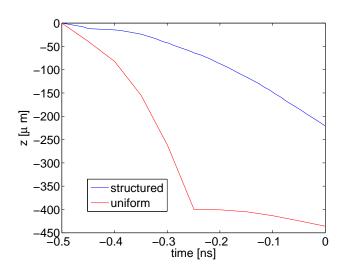


evolution of temperature; timing relates to the laser pulse maximum at $0\ \mathrm{ps}.$

Foam target - structured model

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





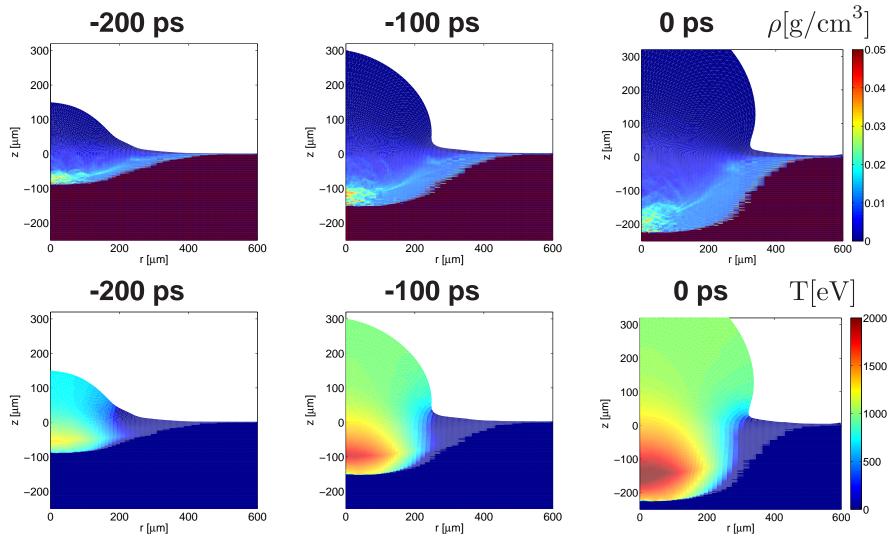
structured foam model

burning of laser through the target

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

Foam target - structured model/2

evolution of density and temperature



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......