Applications of ALE Method to Laser Plasma Studies

R. Liska[1], M. Kuchařík[2], J. Limpouch[1], P. Váchal[1]

[1]Czech Technical University in Prague, Czech Republic
liska@siduri.fjfi.cvut.cz
[2]Los 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 $250ps$, 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**

$$
\begin{aligned}
\frac{d\,\rho}{d\,t} + \rho\,\mathrm{div}\,\mathbf{u} &= 0, \qquad\qquad \frac{d\,\mathbf{x}}{d\,t} = \mathbf{u} \\
\rho\frac{d\,\mathbf{u}}{d\,t} + \mathbf{grad}\,p &= 0 \\
\rho\frac{d\,\epsilon}{d\,t} + p\,\mathrm{div}\,\mathbf{u} &= -\mathrm{div}(\mathbf{I}) + \mathrm{div}(\kappa\mathbf{grad}\,T)
\end{aligned}
$$

- **total Lagrangian time derivatives include convective terms**

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

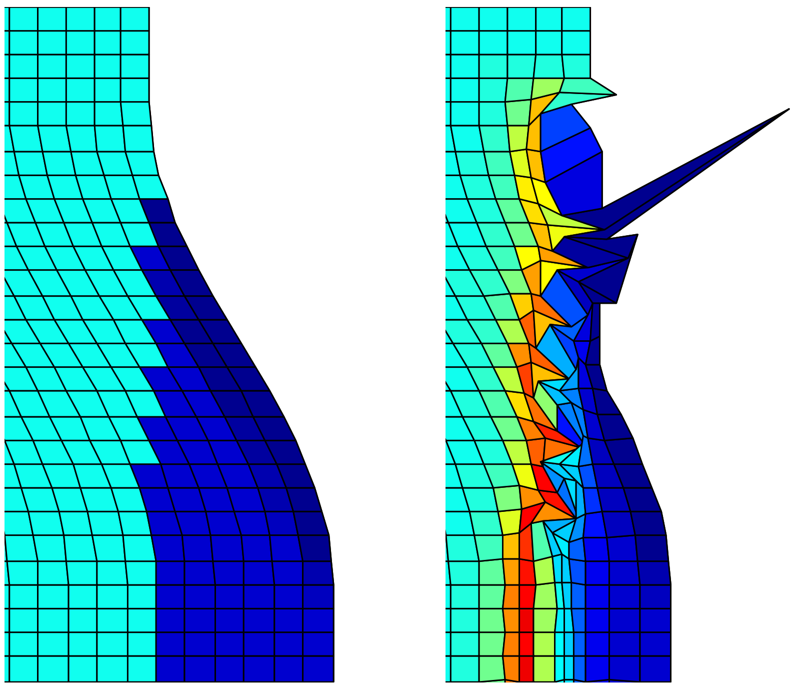
- **equation of state – ideal gas and QEOS for plasma**

- **splitting – hyperbolic and parabolic part**

- **heat conductivity essential – faster shock wave**

Moving Lagrangian Mesh

- moving mesh can **degenerate**



initial Lagr ALE

- 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)]
  - 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 smothing [Winslow (1963)]**

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

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)].**

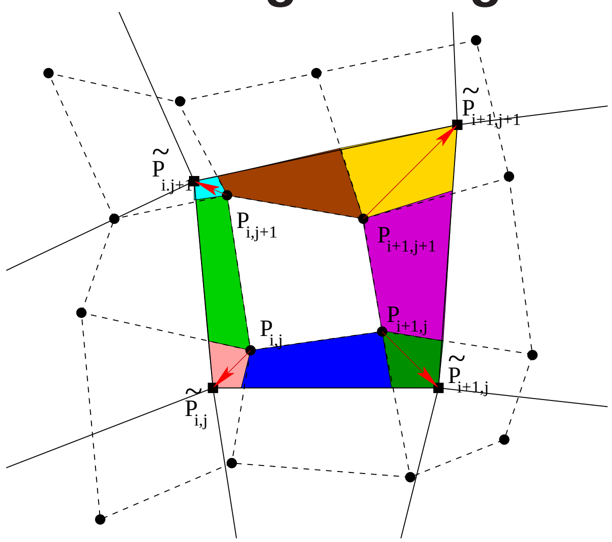
III. Remapping/1

- **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**

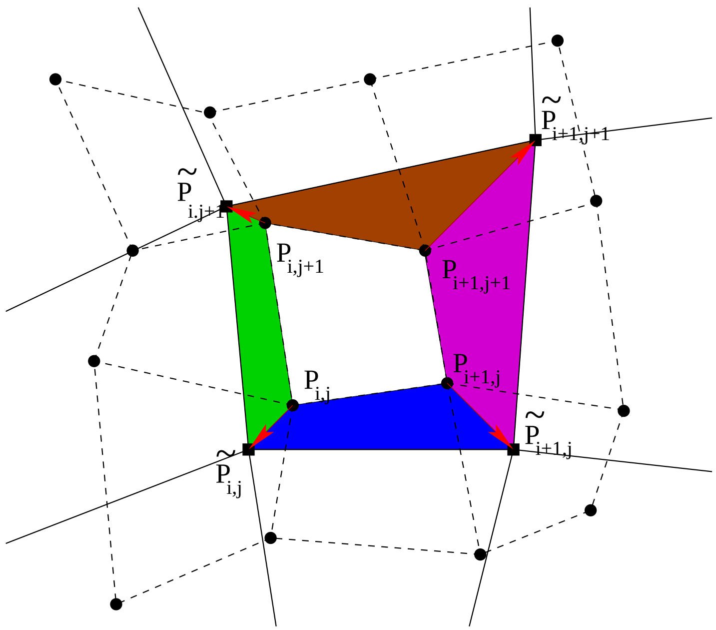


∗ **old mesh dashed, new mesh solid**

∗ **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**

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

- **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**
- **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 $aT_t + \mathrm{div}\mathbf{w} = 0, \mathbf{w} = -\kappa\, \mathbf{grad}\, T = 0$ 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
$$\begin{aligned} a\frac{T^{n+1} - T^n}{\Delta t} + D\mathbf{W}^{n+1} &= 0 \\ \mathbf{W}^{n+1} - GT^{n+1} &= 0 \end{aligned}$$

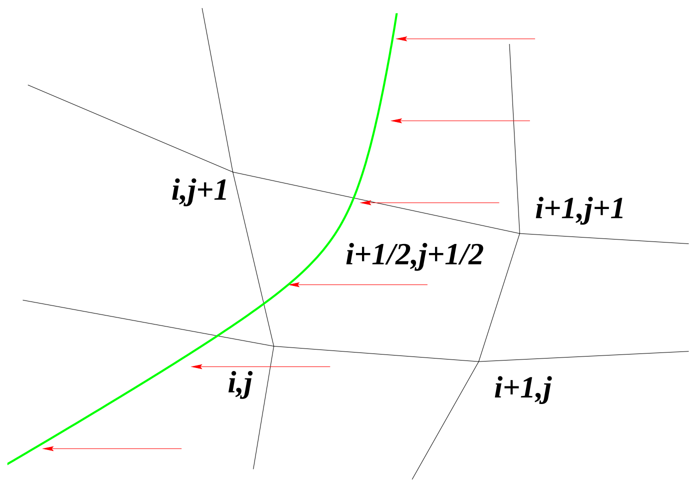
- temperature T^{n+1} is eliminated and the system is solved for heat flux $\mathbf{W}^{n+1}$; the matrix of the system is symmetric and positive definite; same time step as in hyperbolic Lagrangian/ALE step

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

- generalization to cylindrical geometry.

Laser absorption

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

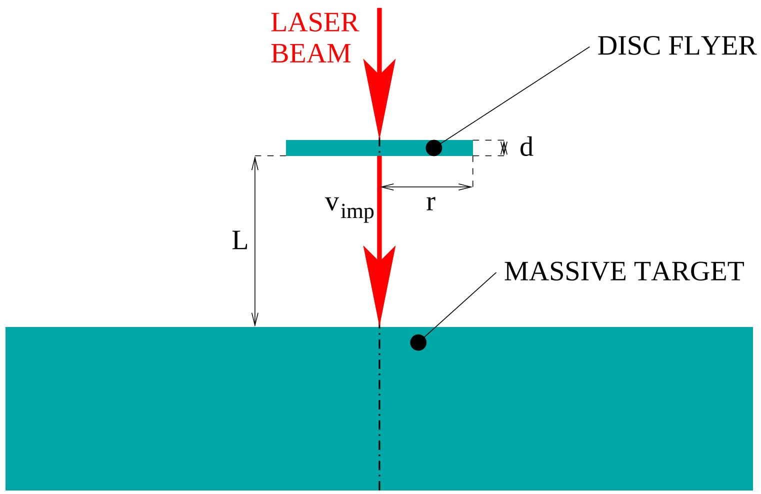


- **source in internal energy equation** $\rho\frac{d\,\epsilon}{d\,t} + p\,\mathrm{div}\,\mathbf{u} = -\mathrm{div}(\mathbf{I})$

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

High velocity impact

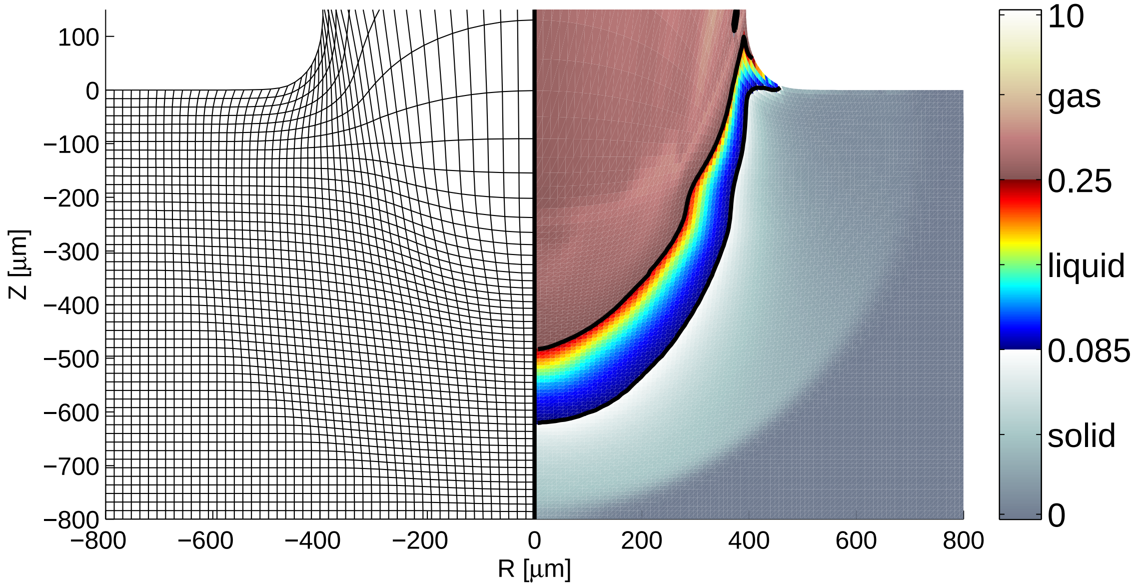
- disc flyer impact problem
- high power laser-irradiated Aluminum disc ablatively accelerates up to very high velocity (40-190 km/s) and strikes to massive Aluminum target
- $d = 6; 11\mu m, r = 150\mu m, L = 200\mu m$, laser energy $120 - 390\,\mathrm{J}$, 1-st or 3-rd harmonics, pulse length $400\,\mathrm{ps}$,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

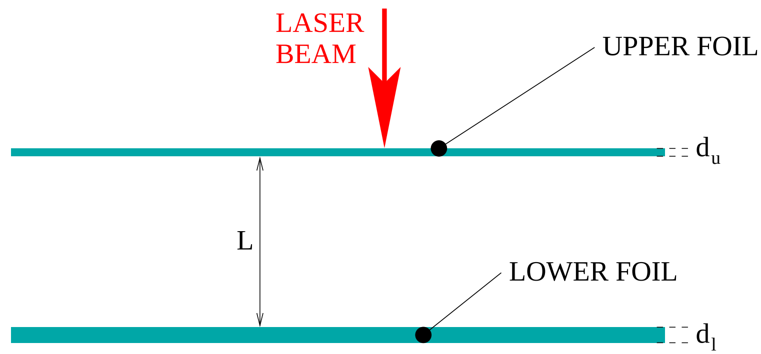


- temperature animation

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

Double foil target

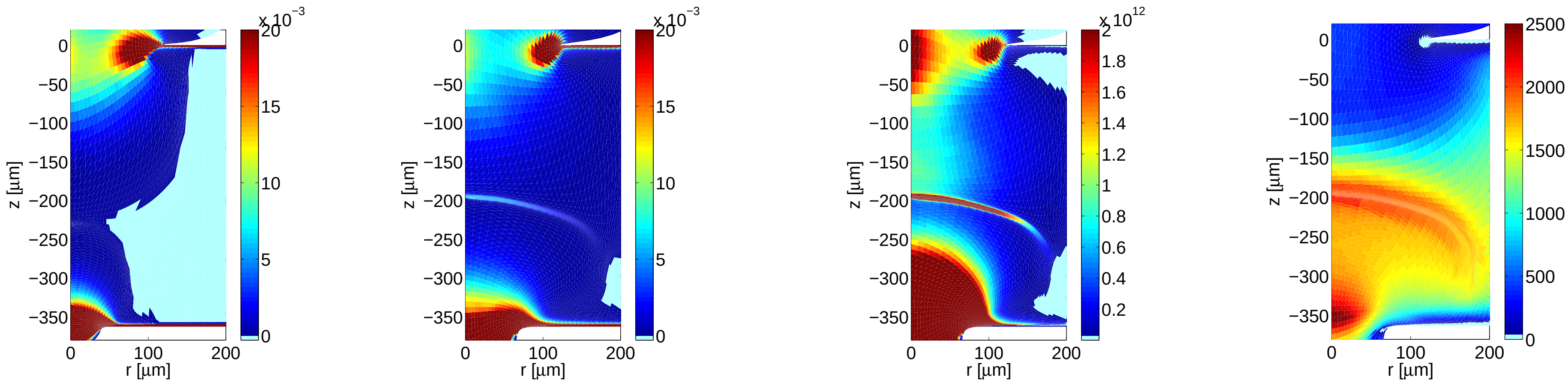
- **foils thickness** $d_u = 0.8\mu m, d_l = 2\mu m$
- **foils distance** $L = 360\mu m$
- **laser energy** $78\,\mathrm{J}$**, 3-rd harmonics, pulse length** $250\,\mathrm{ps}$**, focus** $r_f = 40\,\mu\mathrm{m}$
- **almost vaccum between foils**



- **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**



$\rho[g/cm^3]$ **at 0 ps** $\rho[g/cm^3]$ **at 100 ps** $p[g/(s^2cm)]$ **at 100 ps** $T[eV]$ **at 100 ps**

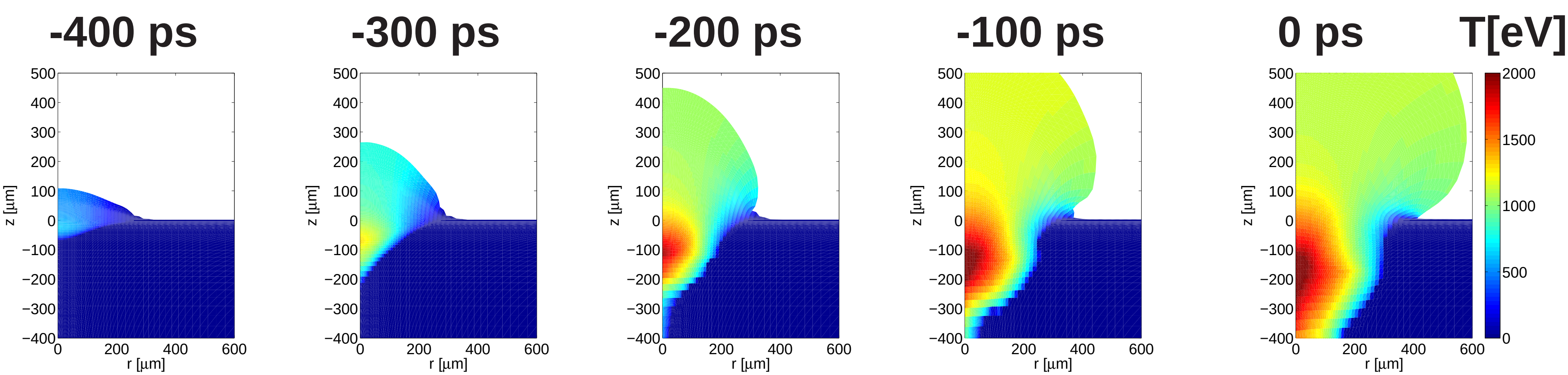
- **double foil target density and pressure animation**

Foam target

- 400μ 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** $320\,\mathrm{ps}$**.**

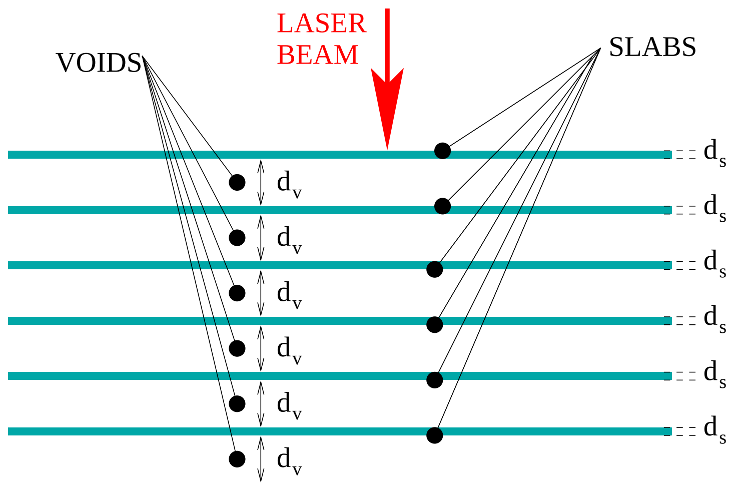
- **foam modelled by uniform density** $9.1\mathrm{mg/cm}^3$ **material**



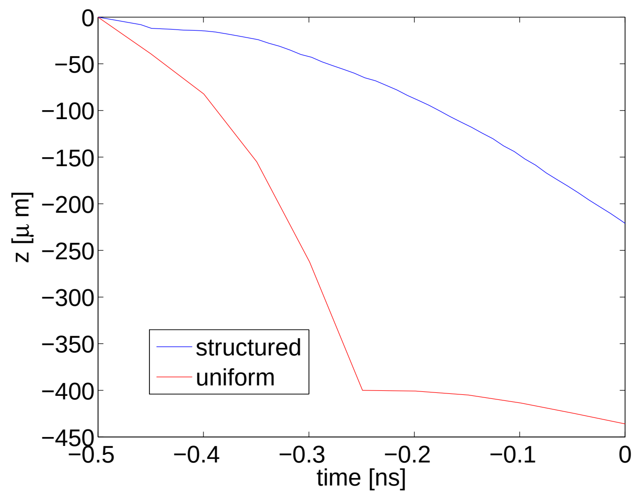
evolution of temperature; timing relates to the laser pulse maximum at $0\,\mathrm{ps}$**.**

Foam target - structured model

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



structured foam model



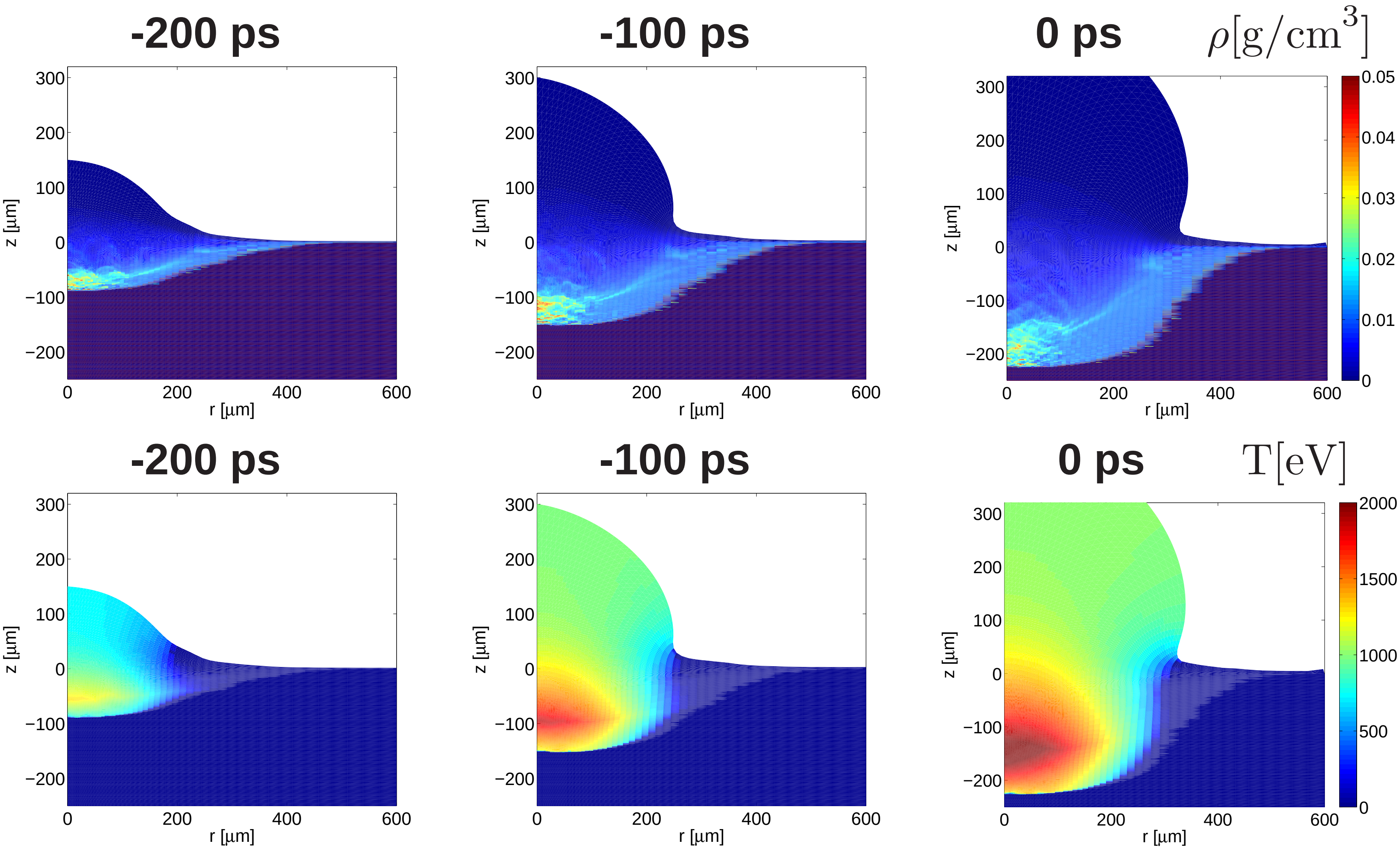
burning of laser through the target

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