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Hydrodynamic Simulations of LPP

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IMPULSE

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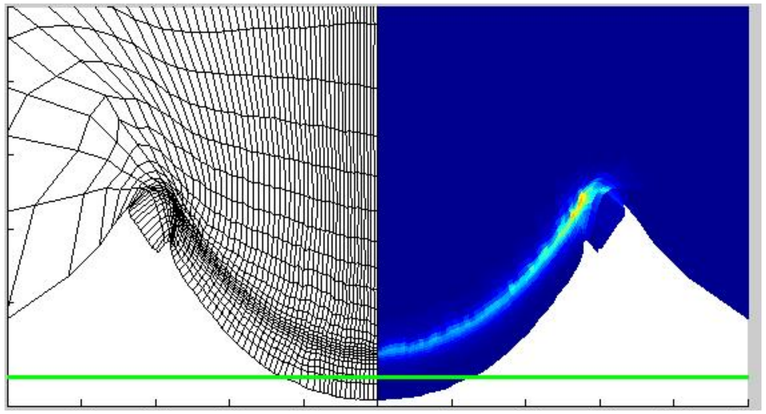
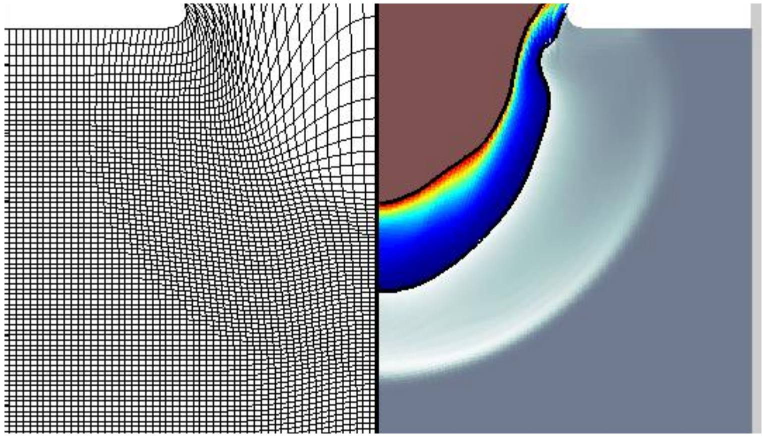
Overview

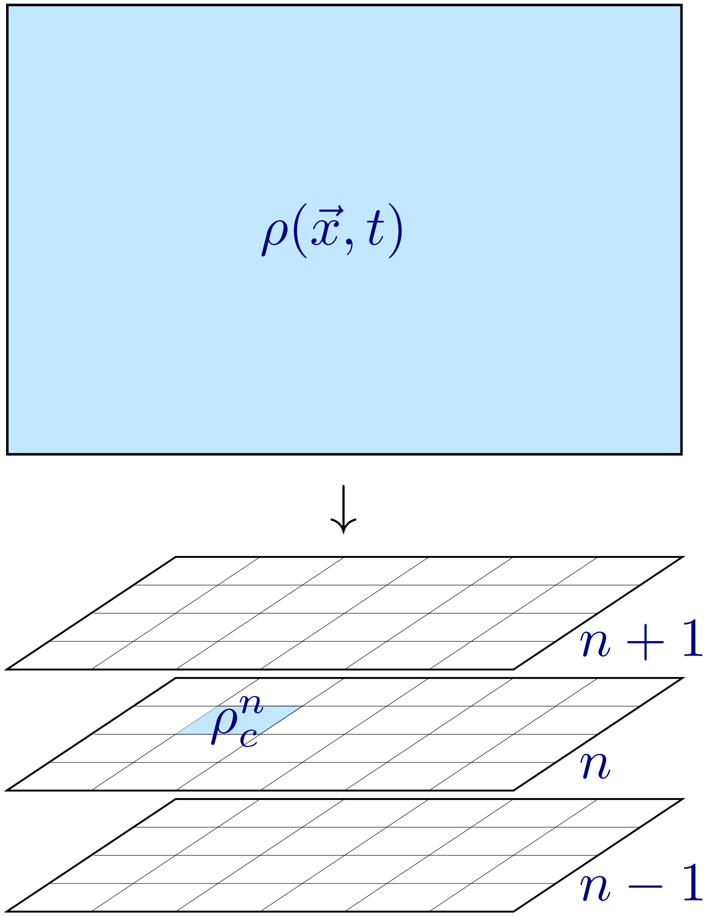
- Hydrodynamic simulations.
- Euler equations in Eulerian and Lagrangian frameworks.
- Eulerian × Lagrangian × ALE methods.
- Indirect Arbitrary Lagrangian-Eulerian (ALE) methods.
- Physical models for LPP.
- Examples of hydrodynamic LPP simulations.
- Conclusions.





Hydrodynamic (fluid) simulations

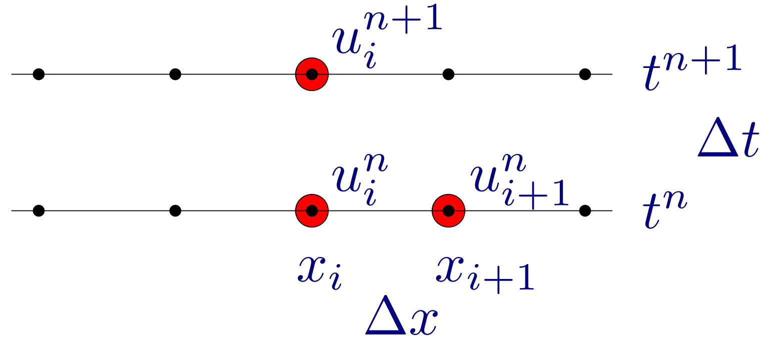
- Hydrodynamics = dynamics of fluids.
- Use: setup of experiments, suitable parameters, interpretation of experiments, . . .
- Description of fluid by (hyperbolic) PDEs, solution by tools of Computational Fluid Dynamics.
- Fluid properties represented by macroscopic quantities – density, velocity, pressure, specific internal energy, . . .
- Discretization:
  - space: computational mesh, cells c;
  - time: sequence of meshes, time levels n.
- Approximation of continuous density (other quantity) function $\rho(\vec{x}, t)$ by its discrete values $\rho_c^n = \rho(\vec{x}_c, t^n)$.



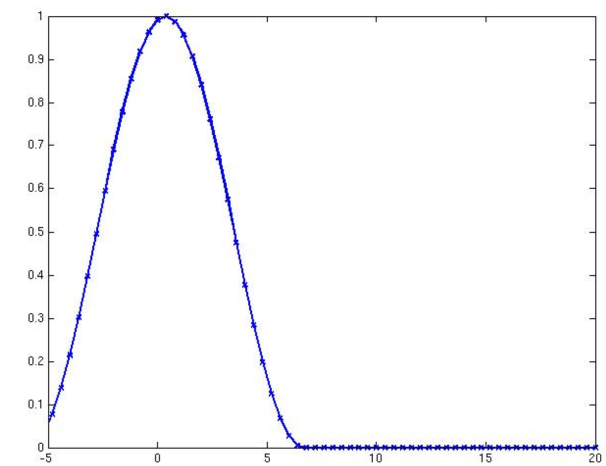
- Transformation of PDEs for $\rho(\vec{x}, t)$ to system of algebraic equations for ρ_c^n.

Example: Finite difference method in 1D

- Advection equation – simplest hyperbolic PDE: $\frac{\partial u}{\partial t} + a\,\frac{\partial u}{\partial x} = 0$.
- Continuous space / time (x,t) discretized by series of meshes (x_i, t^n), i spatial index, n temporal index.



- Approximating derivatives by finite differences: $\frac{\partial u}{\partial x} = \lim_{h\to 0} \frac{u(x+h)-u(x)}{h} \approx \frac{u_{i+1}-u_i}{\Delta x}$
- All derivatives – numerical scheme: $\frac{u_i^{n+1}-u_i^n}{\Delta t} + a\,\frac{u_{i+1}^n-u_i^n}{\Delta x} = 0$.
- Various differences – various schemes – various properties.
- Solving the scheme – update of quantities: $u_i^{n+1} = u_i^n - a\,\frac{\Delta t}{\Delta x}\left(u_{i+1}^n - u_i^n\right)$.
- Other possibilities: finite volumes, finite elements, . . .
- Always approximate !



Euler equations

- Simplest approximation – Euler equations.
- System of hyperbolic PDEs representing conservation of mass, momentum, and total energy:

$$\rho_t + \mathrm{div}(\rho\,\vec{w}) = 0\,, \tag{1}$$

$$(\rho\,\vec{w})_t + \mathrm{div}(\rho\,\vec{w}^2) + \overrightarrow{\mathrm{grad}}\;p = 0\,, \tag{2}$$

$$E_t + \mathrm{div}(\vec{w}\,(E+p)) = 0\,. \tag{3}$$

- Here: ρ – density, $\vec{w}$ – velocity, p – pressure, $E = \rho\,\varepsilon + \frac{1}{2}\rho\,|\vec{w}|^2$ – total energy density, ε – specific internal energy.
- More unknowns than equations – system enclosed by equation of state (EOS): $p = \mathcal{P}(\rho, \varepsilon)$. Ideal gas – $p = (\gamma - 1)\,\rho\,\varepsilon$, where γ – gas constant (ratio of its specific heats).
- General fluid (plasma) – complicated (non-linear) EOSes, often tabulated.

Transformation from Eulerian to Lagrangian framework

- Transforming system to moving (Lagrangian) reference frame.
- Example – conservation of mass in 1D: $\rho_t + (\rho\, u)_x = 0$, expanding derivative: $\rho_t + u\, \rho_x + \rho\, u_x = 0$.
- This can be written as $\frac{D\,\rho}{D\,t} + \rho\, u_x = 0$, where $\frac{D}{D\,t} = \frac{\partial}{\partial t} + \frac{\partial x}{\partial t}\frac{\partial}{\partial x} = \frac{\partial}{\partial t} + u\,\frac{\partial}{\partial x}$ is the Lagrangian (total, material) derivative.
- In multiD: $\frac{D}{D\,t} = \frac{\partial}{\partial\, t} + \vec{w} \cdot \nabla$.
- Similarly for the whole system:

$$\frac{D\,\rho}{D\,t} + \rho\,\nabla \cdot \vec{w} = 0\,, \tag{4}$$

$$\rho\,\frac{D\,\vec{w}}{D\,t} + \nabla\, p = \vec{0}\,, \tag{5}$$

$$\rho\,\frac{D\,\varepsilon}{D\,t} + p\,\nabla \cdot \vec{w} = 0\,. \tag{6}$$

Euler equations – notes

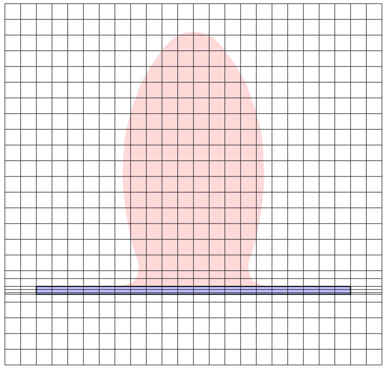
- Eulerian form – usually for conservative quantities, Lagrangian form – usually for primitive quantities, equivalent.

- Inter-connected system of PDEs $\rightarrow$ cannot be solved analytically (except for few special cases) $\Rightarrow$ numerical methods.

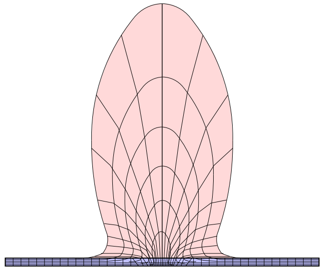
- Remains to define IC ($\rho(\vec{x}, t = 0) = \rho_0(\vec{x})$) and BC (wall, free, periodic, physics dependent, . . .) – can be most difficult.

- Can be solved in both formulations.

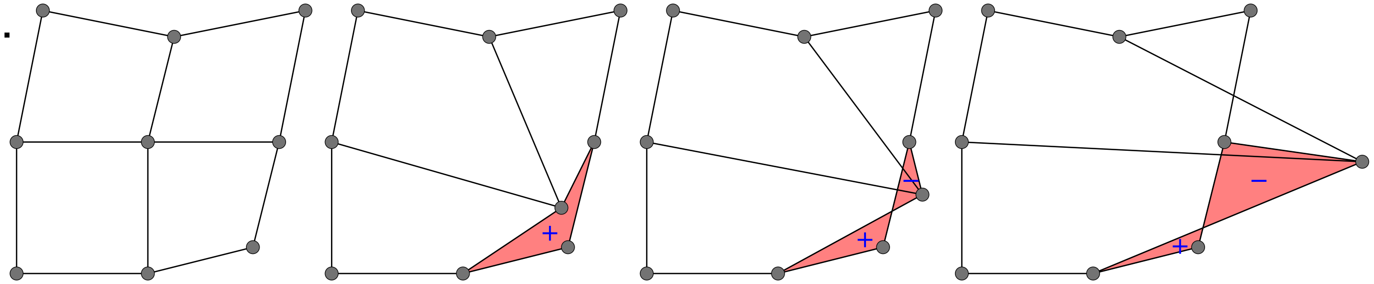
Eulerian vs. Lagrangian methods



- Eulerian methods:
  - Fixed computational mesh, not changing in time.
  - Fluid moves between mesh cells in the form of mass fluxes.
  - Simpler methods, easier to analyze.
  - Problem: Not suitable for highly-volume-changing problems – typical in laser/plasma simulations, where strong material compressions and expansions occur.



- Lagrangian methods:
  - Computational mesh moves naturally with the fluid.
  - No mass fluxes, constant masses in cells.
  - Optimal for strongly changing domains.
  - Problem: Due to mesh motion, mesh can degenerate – non-convex, self-intersecting, or completely inverted cells $\rightarrow$ increase of numerical error or simulation failure.



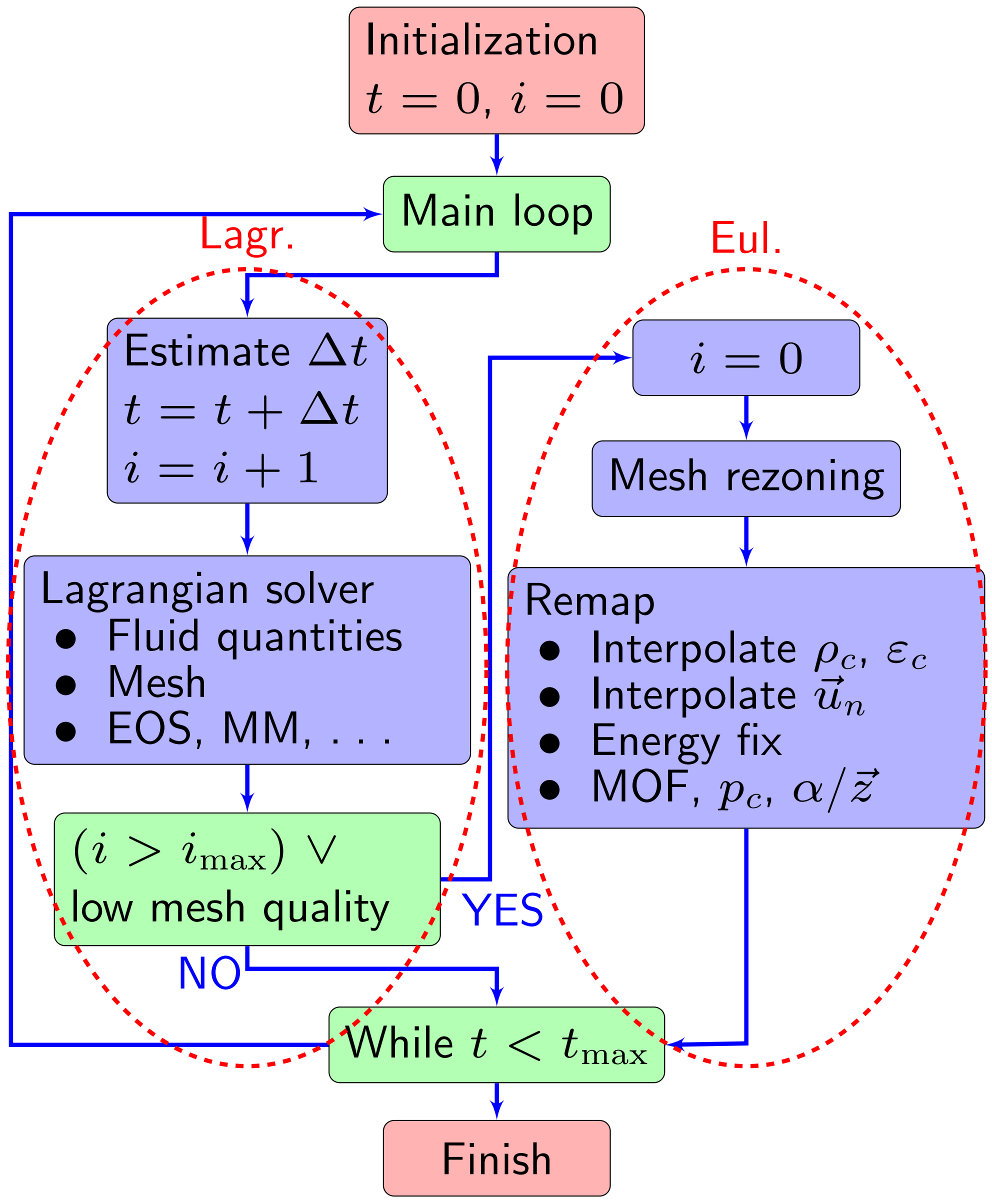
Arbitrary Lagrangian-Eulerian (ALE) methods

- Combination of both approaches – mesh following the fluid motion + guarantee its validity[1].
- Recently very popular, present in many hydrodynamic laser/plasma codes.
- 2 types: direct vs. indirect ALE.
- Direct ALE methods:
  - Separate fluid and mesh velocities.
  - More complicated equations – formulation of fluid flow on differently moving mesh $\rightarrow$ convective term representing mass flux.
  - Filtering dangerous velocity components (shear flow, vortexes) out from the velocity field.

[1] Hirt, Amsden, Cook: JCP, 1974.

Indirect ALE methods

- Explicit separation of 3 steps:
  - 1) Lagrangian step = solver of PDEs, evolution of fluid quantities and mesh in time;
  - 2) Rezoning = untangling and smoothing of computational mesh, increasing its geometric quality;
  - 3) Remap = conservative interpolation of all quantities from Lagrangian to rezoned mesh.
- Rezone + remap = Eulerian part of the ALE algorithm (fluxes).
- Different strategies for triggering rezone/remap on (degeneracy, Eulerian, counter, . . .)



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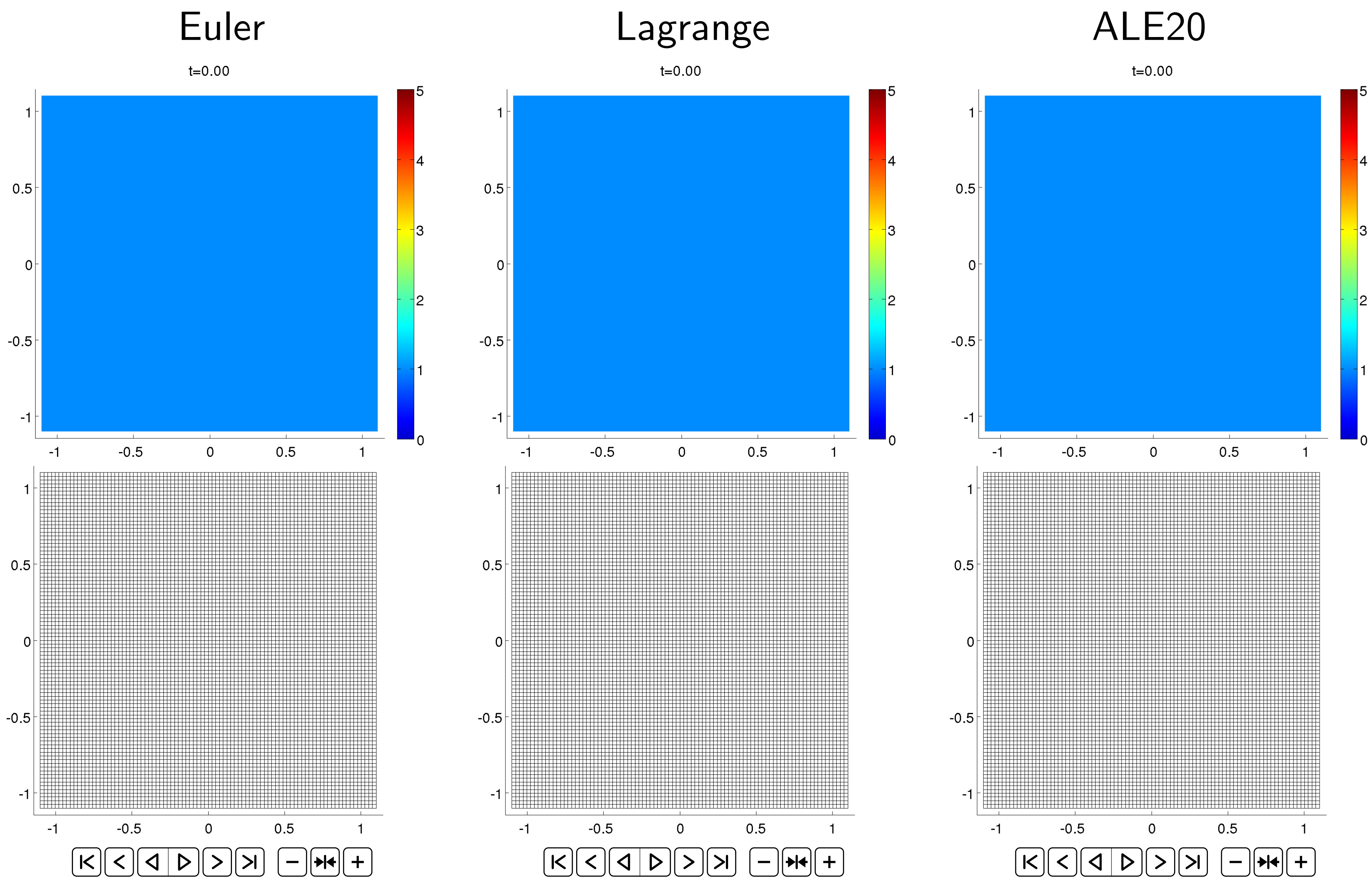
Example: Sedov blast wave



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Physical aspects – Model

- Laser plasma – simplest approximation by modification of energy equation:

$$\frac{D\,\rho}{D\,t} = -\rho\,\nabla\cdot\vec{w}\,, \tag{7}$$

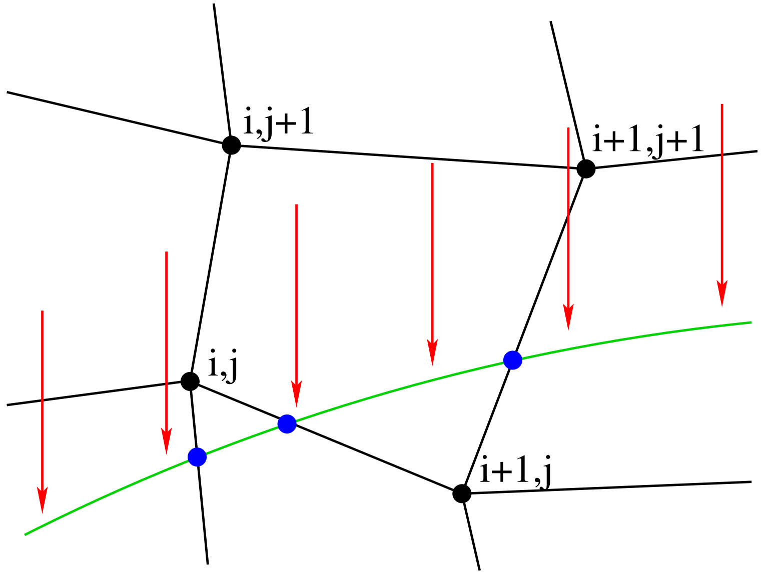
$$\rho\,\frac{D\,\vec{w}}{D\,t} = -\nabla\,p\,, \tag{8}$$

$$\rho\,\frac{D\,\varepsilon}{D\,t} = -p\,\nabla\cdot\vec{w} + \nabla\cdot(\kappa\nabla T) - \nabla\cdot\vec{I}\,, \tag{9}$$

where T is temperature, κ is heat conductivity coefficient, and $\vec{I}$ is laser beam intensity profile.

Physical aspects – Laser absorption

- Various models based on geometrical × wave optics.
- Simple model of laser absorption on the critical surface[1].
- Approximation of $(D\,\vec{I})_c$ in critical cells, $(D\,\vec{I})_c = 0$ in sub- or super-critical cells.
- Equation of absorption: $\rho \frac{D\,\varepsilon}{D\,t} + p\,\nabla \cdot \vec{w} = -C_A\,\nabla \cdot \vec{I}$, C_A – absorption coefficient.
- Problems – C_A needed from user + full absorption in one cell → series of "cell explosions".



- More advanced models.
- Raytracing[2] – explicit tracking of each single ray in the domain, including its refractions on the cell boundaries.
- Wave-based models employing stationary solution of Maxwell equations[3].

[1] Liska, Kucharik: EQUADIFF, 2007.
[2] Chaudhury, Chaturvedi: PoP, 2006.
[3] Kapin, Kucharik, Limpouch, Liska: CzJP, 2006.

Physical aspects – Heat conductivity

- Represented by parabolic term in the energy equation.
- Operator splitting → separate parabolic PDE in temperatures, $T_t = \frac{1}{\rho\,\varepsilon_T} \nabla \cdot (\kappa \nabla T)$.
- Typically classical Spitzer-Harm heat conductivity coefficient $\kappa \approx T^{5/2}$.
- Approximation[1] of gradient and divergence by discrete operators G, D.
- Typically implicit scheme in time $(T^{n+1} - T^n)/\Delta t + D\,G\,T^{n+1} = 0$, explicit not suitable: CFL ⇒ many steps per 1 Lagrangian step.
- Numerical heat flux can be higher than physically feasible – limiter needed.
- Usually: 1) solve → $W^{\rm num}$, 2) renormalize $\tilde{\kappa} = f^{\rm max} \frac{W^{\rm lim}}{W^{\rm num}} \kappa$, where the coefficient $f^{\rm max} \in (0.05, 0.3)$, 3) solve again with modified $\tilde{\kappa}$.
- Need to solve system twice → new temperatures/energies more realistic.

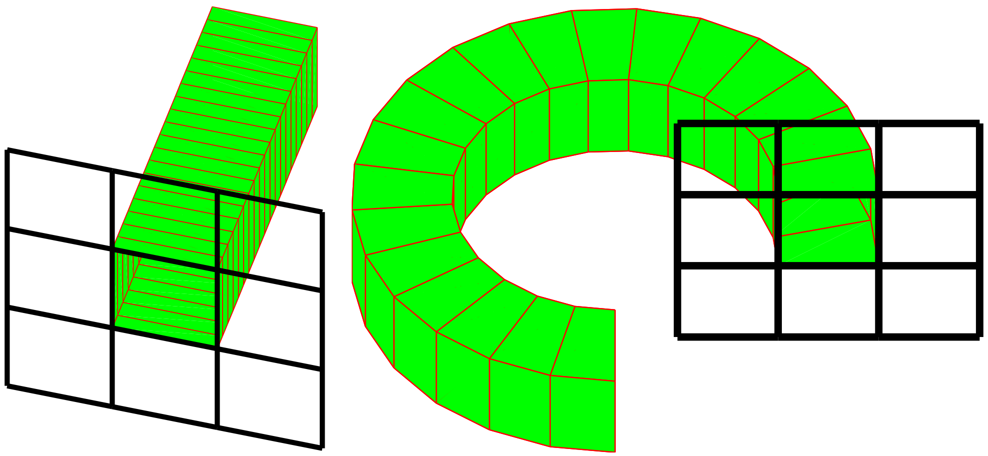
[1] Shashkov, Steinberg: JCP, 1996.

Physical aspects – EOS

- EOS crucial, strongly affects realistic simulations.
- Ideal gas for simple fluid test, reasonably valid in low-density corona.
- Realistic EOSes – significantly more computationally expensive, often tabulated.
- Quotidian EOS (QEOS)[1] for real plasma – Thomas-Fermi theory for electrons and Cowan model for ions.
- Sesame EOS[2] – tables of measured values + several material theories providing interpolation techniques.
- Various modifications – such as Badger or FEOS.
- HerEOS[3] – library for Hermite interpolation of tabulated data.

[1] More, Warren, Young, Zimmerman: PF, 1988.
[2] Lyon, Johnson: LANL Report, 1992.
[3] Zeman, Holec, Vachal: CMA, 2019.

Physical aspects – ALE in cylindrical geometry



- Many laser-related processes are cylindrically symmetrical, 2D code with cylindrical geometry well approximates 3D reality.
- Switching to cylindrical geometry = adding r factor into all integrals – different volumes, centroids.
- Lagrangian solver – adding r factor leads to Control Volume scheme: integration mainly in forces.
- Mesh rezoning – no change, done as in Cartesian case.
- Remap: r arises during integration.

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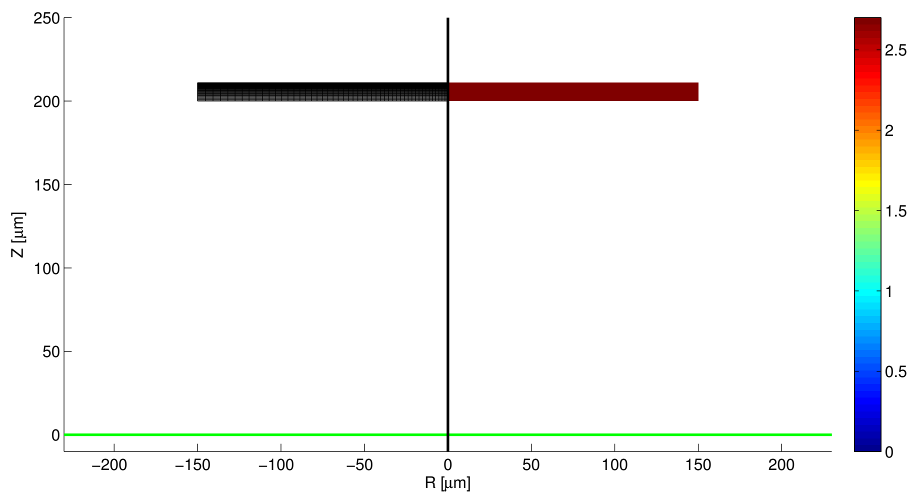
Physical aspects – Others

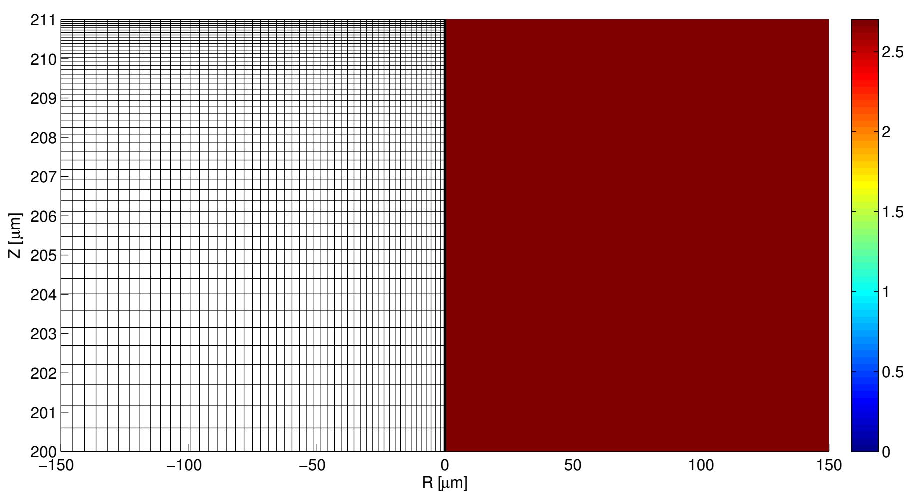
- Many other models can be needed/usefull:
  - Two-temperature model – separate electron/ion temperatures $\rightarrow$ two energy equations + heat exchange term. More realistic for non-ideal plasma.
  - Phase transition model – taking into account latent heat of melting and evaporation, important for interaction with solid targets.
  - Non-local energy transport – represents long-distance transfer of energy due to material radiation.

- Our group develops Prague ALE (PALE) code – simulations of laser/target interactions, experiments at PALS or ELI.

Example 1: Disc target acceleration

- Simulation inspired by experiments on PALS system[1].
- Laser evaporates disc target, acceleration to tens/hundreds km/s[2].





- Geometrical computational mesh, in disc only.
- Laser absorption, material evaporation upwards. Massive part of the disc accelerated downward due to ablation (momentum conservation).
- Experimental disc velocity compared with simulations[3], good agreement.

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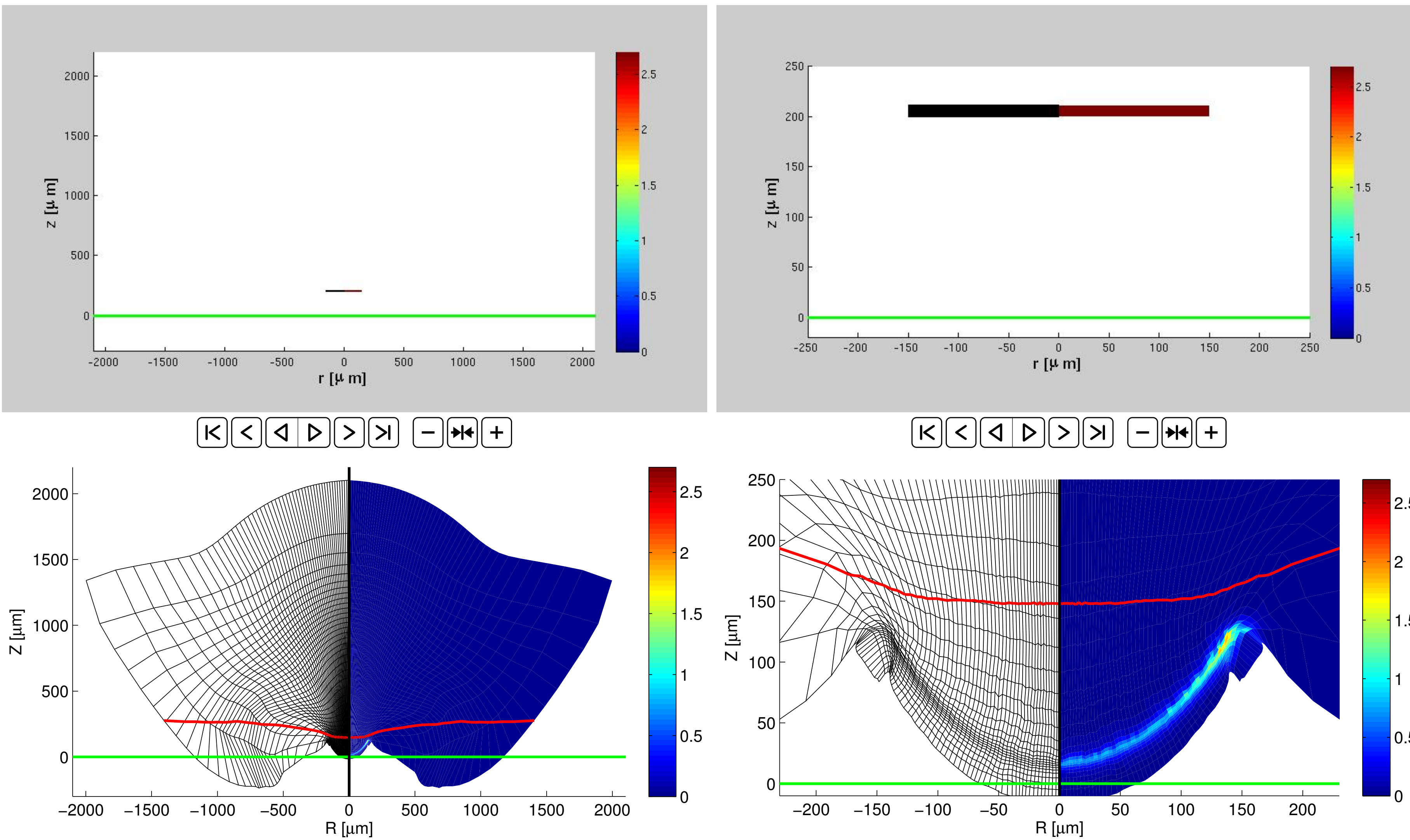
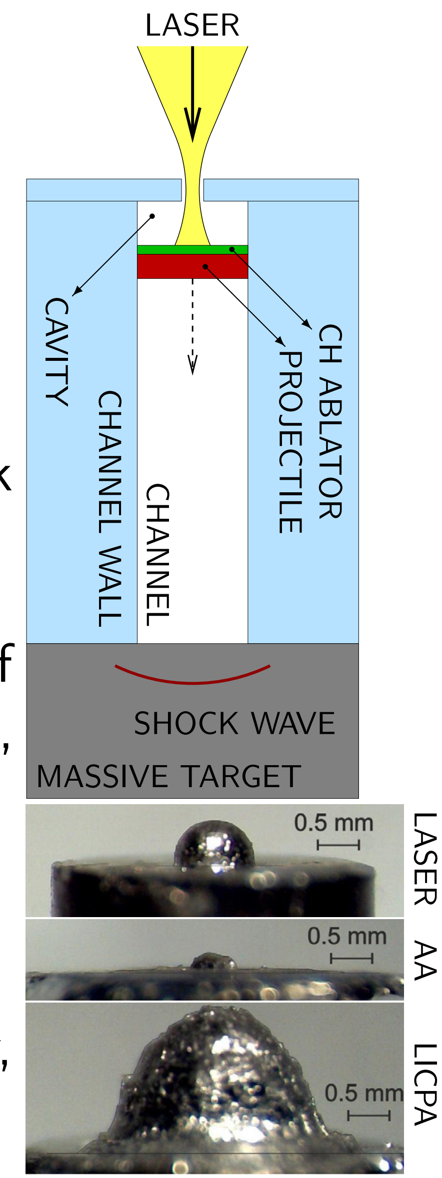
[1] Borodziuk, Kasperczuk, Pisarczyk, et al.: CzJP, 2003.
[2] Kalal, Borodziuk, Demchenko, et al.: ECLIM, 2004.
[3] Kucharik, Limpouch, Liska, Havlik: ECLIM, 2004.

Example 1: Disc target acceleration



Example 2: LICPA scheme

- Laser induced cavity pressure acceleration[1].
- Preparation, analysis, interpretation of PALS experiments.
- Simulations of processes in channel covered by a cavity.
- Cavity ⇒ large portion of laser energy transferred to shock wave ⇒ higher impact velocity, larger craters.
- Many configurations: width of ablator/projectile, material of projectile/target (CH, Al, Cu, Au), laser energy ($100 - 400\,\mathrm{J}$), laser frequency (1ω, 3ω).
- Different aspects of experiments, hydroefficiency.
- Comparison of simulations and experiments (impact velocity, shock speed, crater size) ⇒ reasonably good agreement.



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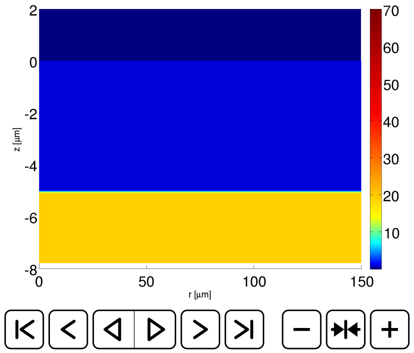
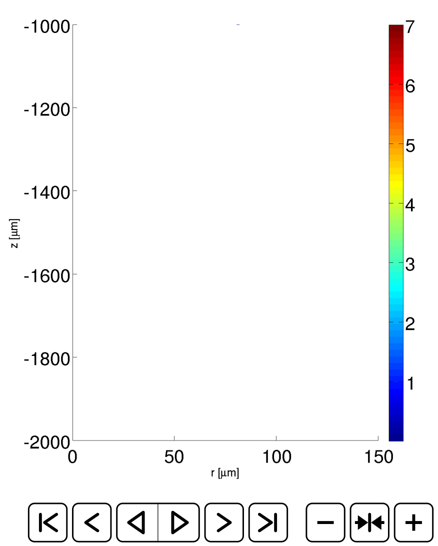
[1] Badziak, Borodziuk, Pisarczyk, et al.: APL, 2010.

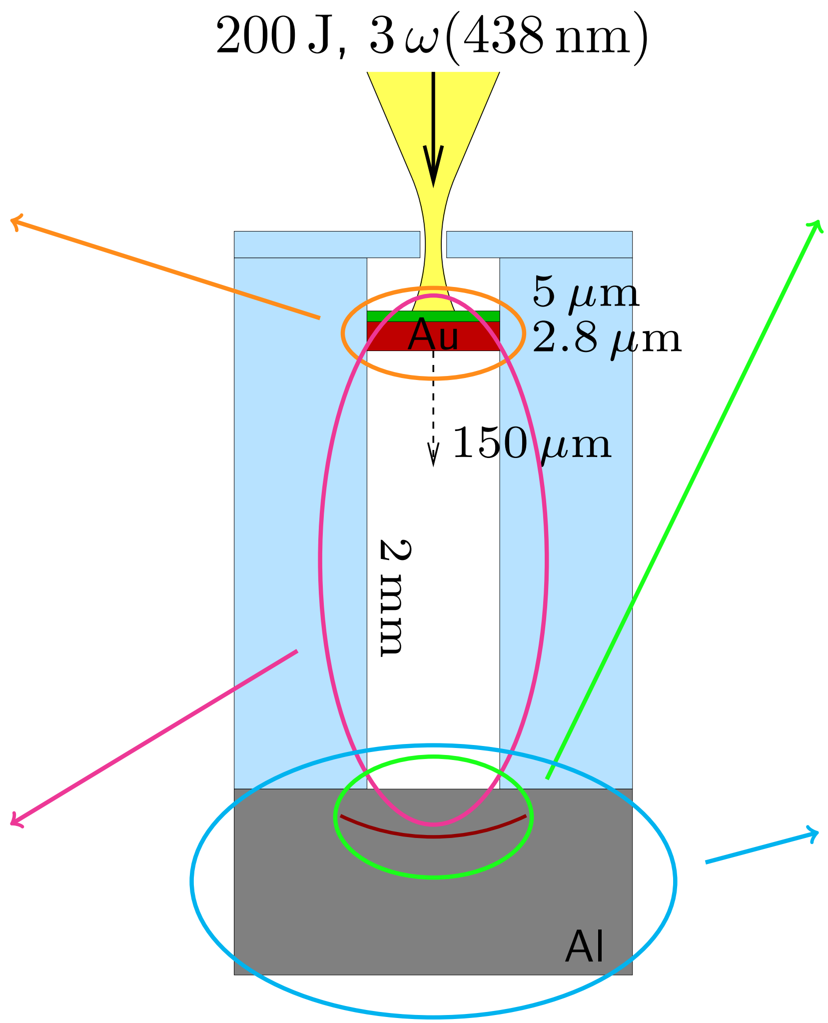
Example 2: LICPA scheme

Absorption

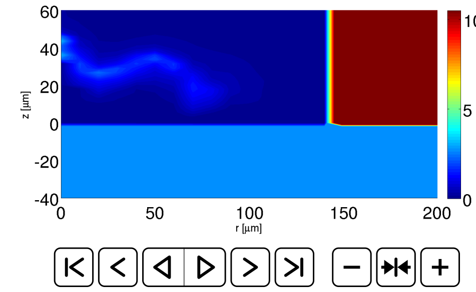


Accel. + impact

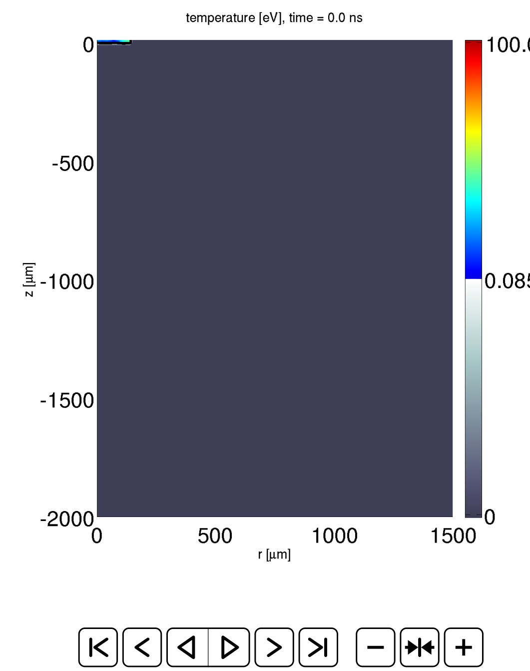




Shock formation



Crater development



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Conclusions

- Hydrodynamic simulations important for understanding of experiments.
- Lagrangian and ALE methods suitable for ICF and laser/target simulations.
- Physical models crucial for realistic results.
- Current codes able to perform realistic laser/target computations.
- Ongoing research, attractive topic.

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