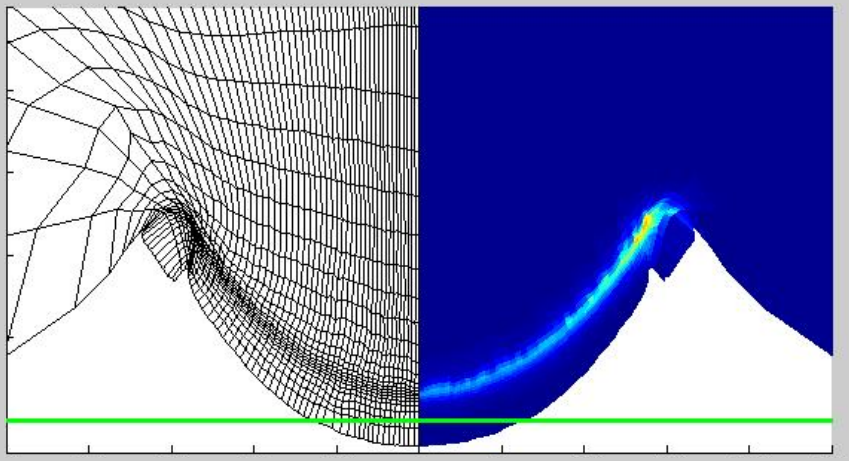

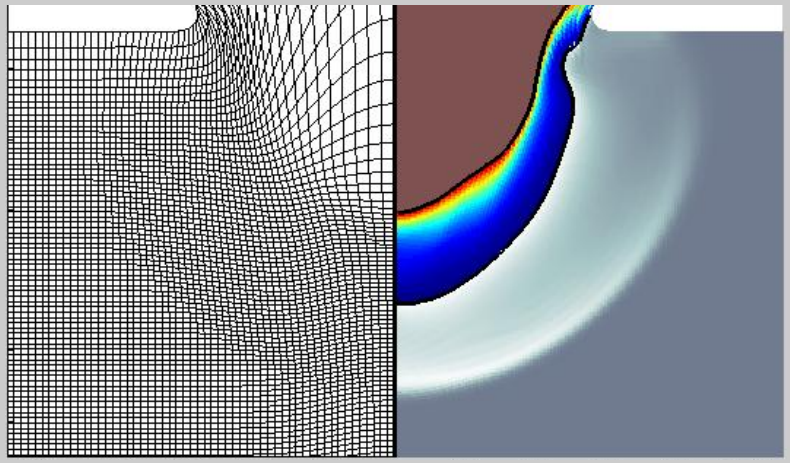

Fluid Simulations for Laser-Produced Plasmas

Milan Kuchařík[†]

[†] Faculty of Nuclear Sciences and Physical Engineering, Czech Technical University in Prague, Břehová 7, Praha 1, 115 19, Czech Republic

milan.kucharik@fjfi.cvut.cz, http://kfe.fjfi.cvut.cz/~kucharik

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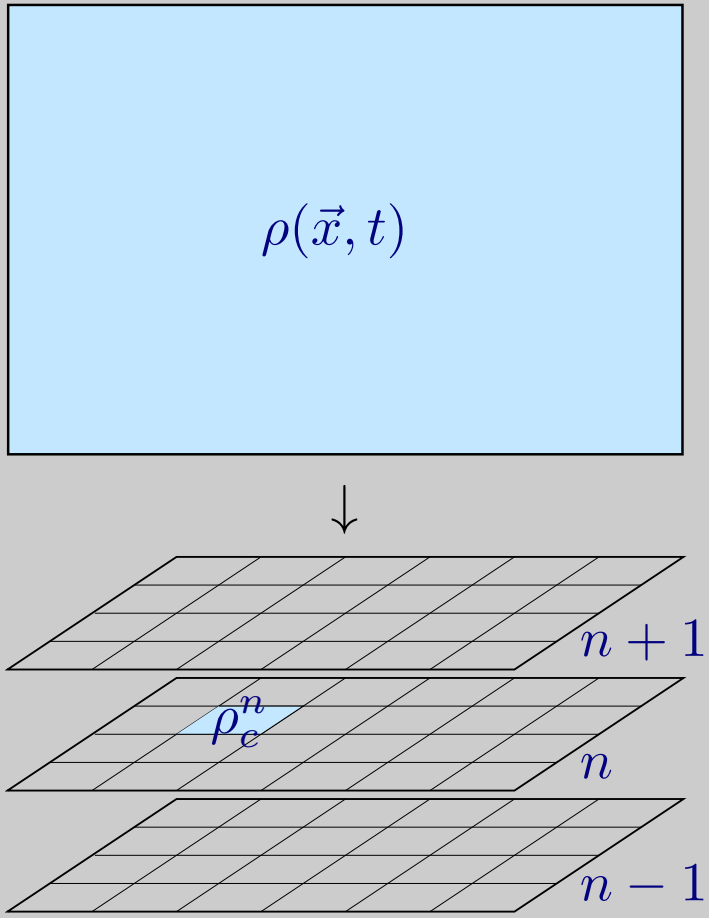
FACULTY OF NUCLEAR SCIENCES AND PHYSICAL ENGINEERING CTU IN PRAGUE

Overview

- Hydrodynamic simulations.
- Euler equations in Eulerian and Lagrangian frameworks.
- Arbitrary Lagrangian-Eulerian (ALE) methods.
- Staggered compatible Lagrangian scheme.
- Mesh rezoning techniques.
- Quantity remapping.
- Physical models for LPP.
- Examples of hydrodynamic ALE simulations.
- Conclusions.

Hydrodynamic (fluid) simulations

- Hydrodynamics = dynamics of fluids.
- Description of fluid by a set of (hyperbolic) PDEs, solution by tools of Computational Fluid Dynamics (CFD).
- 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 system of PDEs for $\rho(\vec{x}, t)$ to system of algebraic equations for ρ_c^n.



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:

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

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

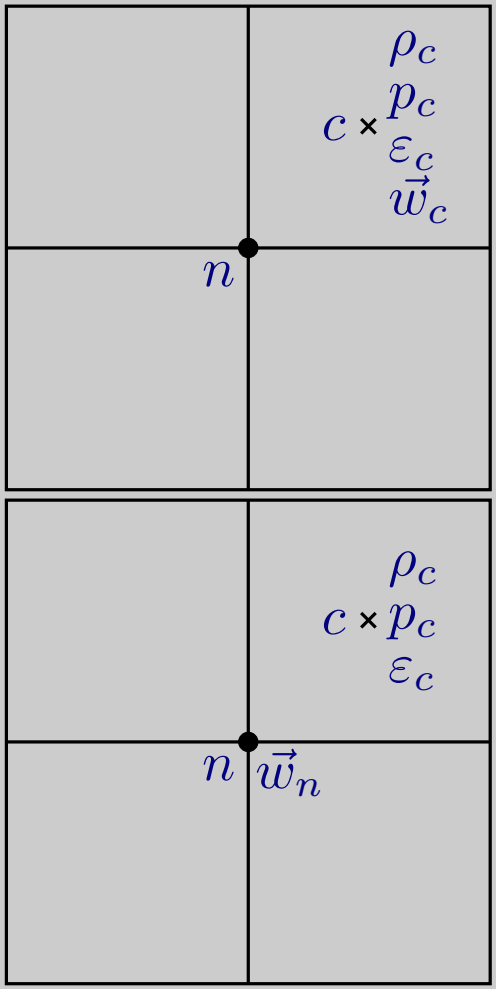
$$\rho\, \frac{D\,\varepsilon}{D\,t} + p\, \nabla \cdot \vec{w} = 0\,. \tag{6}$$

Lagrangian motion

- Motion of Lagrangian particles described by an ODE: $\frac{D\,\vec{x}}{D\,t} = \vec{w}$, typically defines motion of mesh nodes.

- Location of velocity w:
  - in mesh cells $\rightarrow$ cell-centered methods: all quantities located at the same place, need to use approximate Riemann solver at each node to define its velocity;
  - in mesh nodes $\rightarrow$ staggered methods: mesh motion directly defined, different location of thermodynamic (ρ_c, p_c, ε_c) and kinematic ($\vec{w}_n$) quantities.

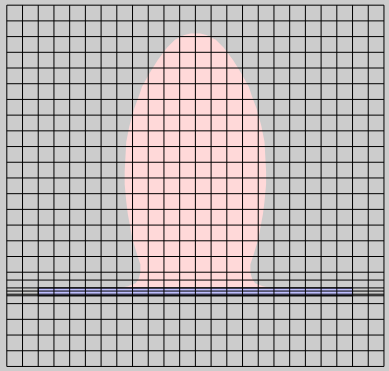
- Computational cells considered to be Lagrangian particles: no mass flux between cells $\Rightarrow$ density given by cell shape (volume), no need to solve mass equation.



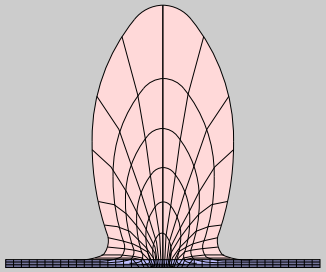
Euler equation – notes

- 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.

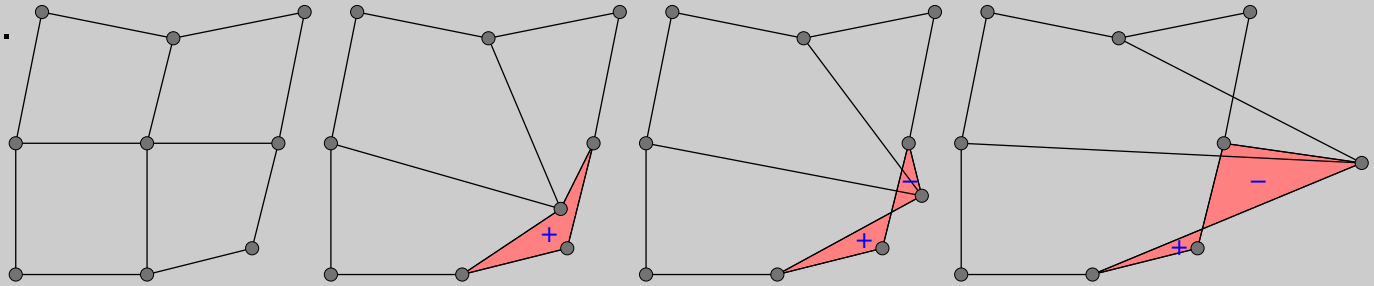
Eulerian vs. Lagrangian methods



- 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.



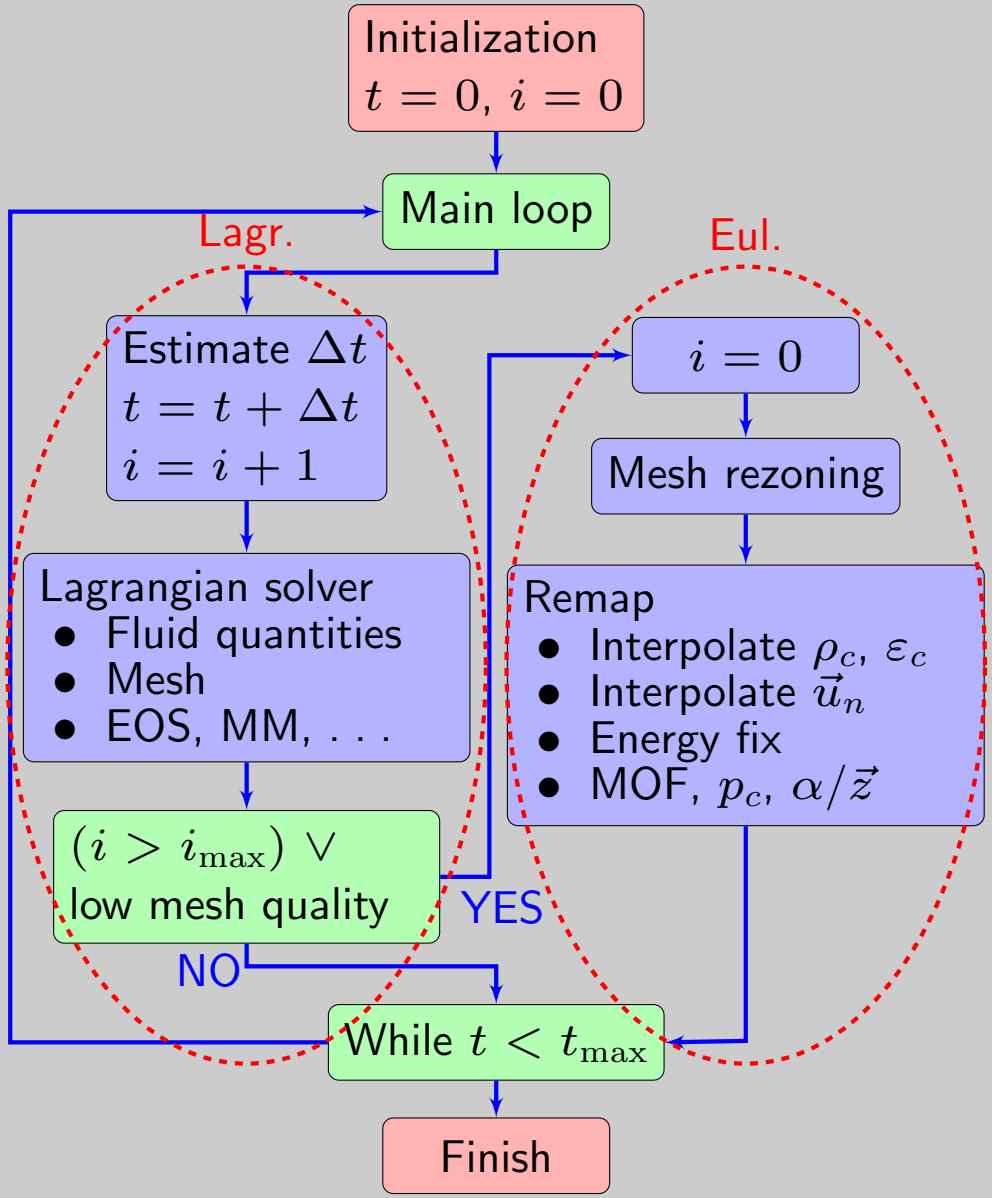
Arbitrary Lagrangian-Eulerian (ALE) methods

- 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.

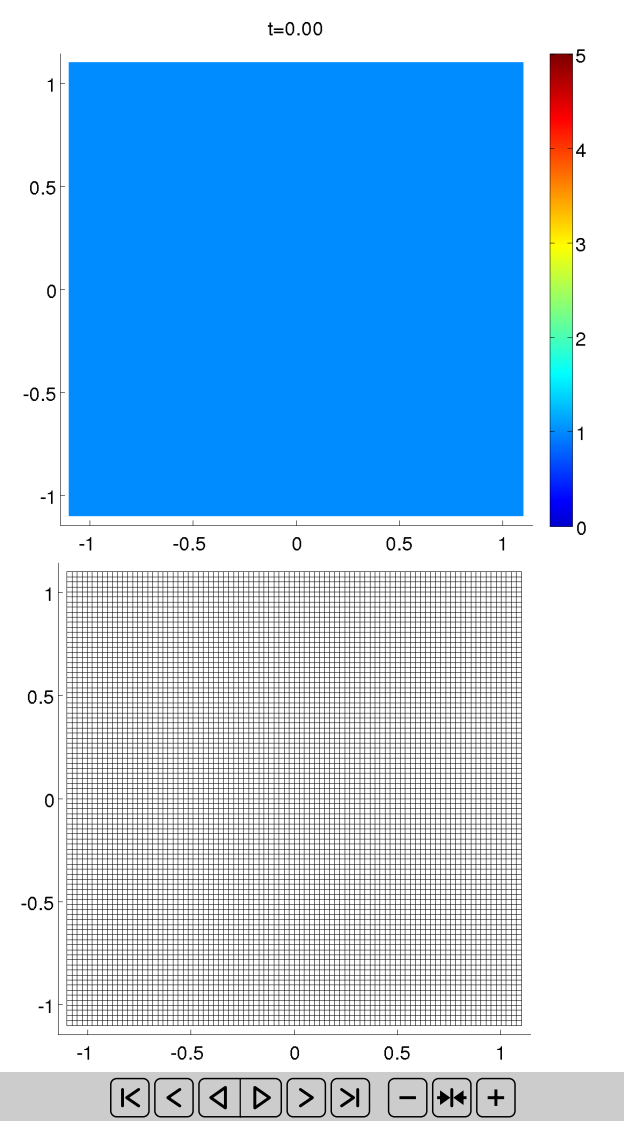
Indirect ALE methods

- 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, . . .)

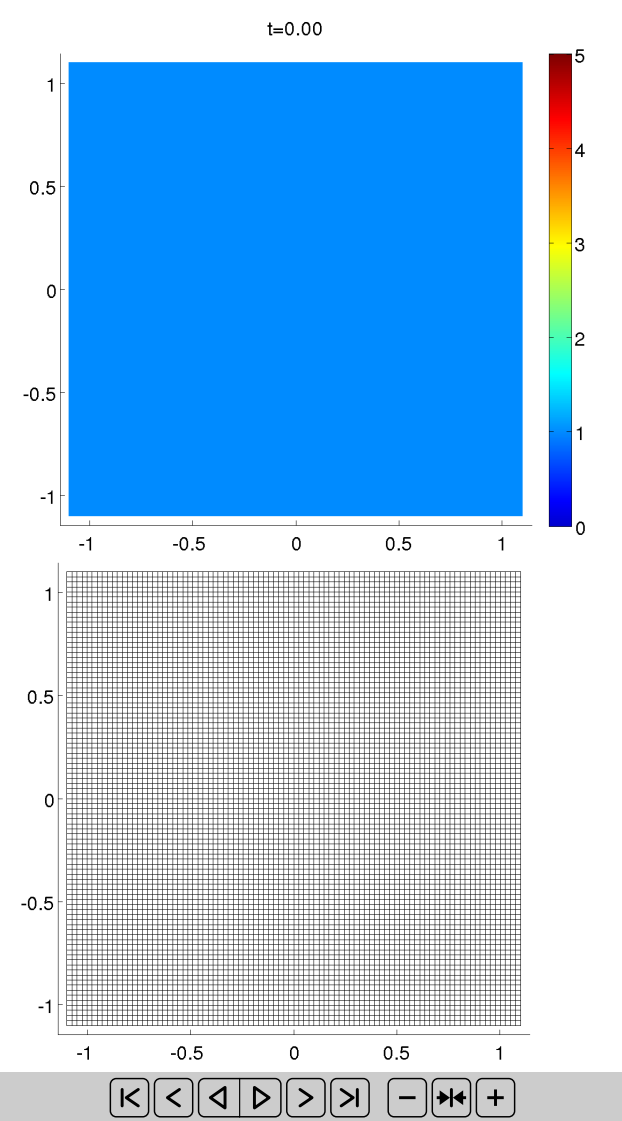


Example: Sedov blast wave

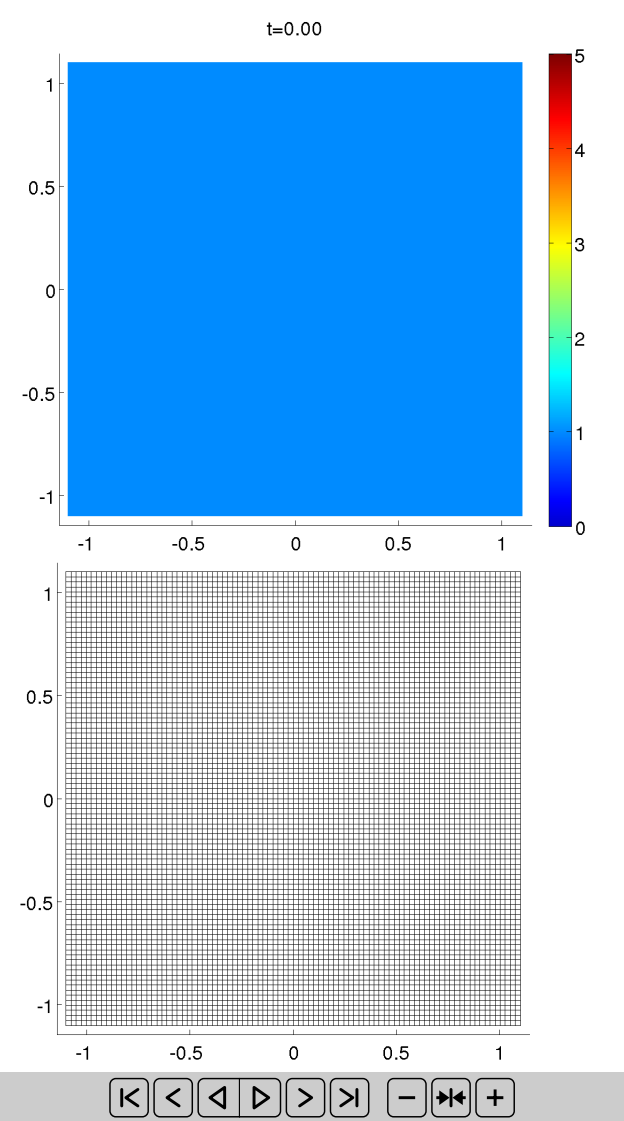
Euler



Lagrange



ALE20



Step 1: Lagrangian solver

- Solving the system of Euler equations in Lagrangian form:

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

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

$$\rho\,\frac{D\,\varepsilon}{D\,t} = -p\,\nabla\cdot\vec{w}\,, \tag{9}$$

with ODE for motion of mesh nodes

$$\frac{D\,\vec{x}}{D\,t} = \vec{w}\,, \tag{10}$$

and equation of state

$$p = \mathcal{P}(\rho,\varepsilon)\,. \tag{11}$$

- Compatible Lagrangian scheme in staggered discretization (mimetic or support operators method)[1].

[1] Caramana, Burton, Shashkov, Whalen: JCP, 1998.

Step 1: Lagrangian solver

- Conservation of mass (7) – constant cell mass $m_c \Rightarrow$ automatically satisfied.

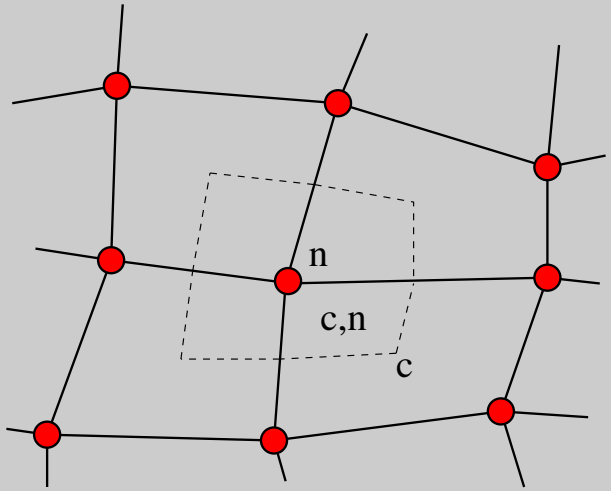
- Integration of momentum equation (8) over dual (nodal) volume V_n,

$$m_n \left(\frac{D\,\vec{w}}{D\,t} \right)_n = \int\limits_{V_n} \rho \frac{D\,\vec{w}}{D\,t}\, dV = - \int\limits_{V_n} \nabla p\, dV \equiv \vec{F}^p_n \,. \tag{12}$$

- Forces on the right hand side can be written as

$$\vec{F}^p_n = \sum_{c \in C(n)} \vec{F}^p_{c,n} \,, \tag{13}$$

where $\vec{F}^p_{c,n}$ is force from cell c to node n due to pressure in c, can be computed from cell pressures and cell geometry.



- Left hand size – approximation of velocity derivative by finite difference:

$$\left. \frac{D\,\vec{w}}{D\,t} \right|_n \approx \frac{\vec{w}_n^{t^{n+1}} - \vec{w}_n^{t^n}}{\Delta t} \quad \Rightarrow \quad \vec{w}_n^{t^{n+1}} = \vec{w}_n^{t^n} + \frac{\Delta t}{m_n} \vec{F}^p_n \,. \tag{14}$$

Step 1: Lagrangian solver

- Motion of computational mesh nodes from (10) – again finite difference

$$\vec{x}_n^{t^{n+1}} = \vec{x}_n^{t^n} + \Delta t\, \vec{w}_n^{t^*} \,. \tag{15}$$

- Computation of new cell volumes $V_c^{t^{n+1}}$ from cell geometry.

- Update of cell densities

$$\rho_c^{t^{n+1}} = m_c / V_c^{t^{n+1}} \,. \tag{16}$$

- Total energy: internal + kinetic:

$$E = \sum_{\forall c} m_c\, \varepsilon_c + \sum_{\forall n} \frac{1}{2} m_n \, \|\vec{w}_n\|^2 = \sum_{\forall c} \left(m_c\, \varepsilon_c + \sum_{n \in N(c)} \frac{1}{2} m_{c,n} \, \|\vec{w}_n\|^2 \right) , \tag{17}$$

where

$$m_c = \sum_{n \in N(c)} m_{c,n} \,, \quad m_n = \sum_{c \in C(n)} m_{c,n} \,. \tag{18}$$

Step 1: Lagrangian solver

- Conservation $\Longrightarrow \partial E/\partial t = 0$, true if in each cell: $\partial E_c/\partial t = 0$,

$$m_c \frac{\partial \varepsilon_c}{\partial t} = - \sum_{n \in N(c)} m_{c,n} \, \|\vec{w}_n\| \, \frac{\partial \|\vec{w}_n\|}{\partial t} \equiv W_c \,. \tag{19}$$

- Substitution for velocity derivative from (12) $\Rightarrow$

$$m_c \frac{\partial \varepsilon_c}{\partial t} = W_c \,, \text{ where } \quad W_c = - \sum_{n \in N(c)} \frac{m_{c,n}}{m_n} \, \vec{w}_n \cdot \vec{F}^p_{c,n} \,. \tag{20}$$

- W_c = released/removed heat in cell c due to its compression/expansion, can be explicitly computed.

- Energy update by central difference again,

$$\varepsilon_c^{t^{n+1}} = \varepsilon_c^{t^n} + \frac{\Delta t}{m_c} W_c \,. \tag{21}$$

- Due to this construction: exact energy conservation up to machine precision.

Step 1: Lagrangian solver

- Remaining only pressure update – from EOS (11),

$$p_c^{t^{n+1}} = \mathcal{P}\left(\rho_c^{t^{n+1}}, \varepsilon_c^{t^{n+1}}\right). \tag{22}$$

- Resulting scheme conservative in mass, momentum, and total energy.

- Usually used in two-step (predictor-corrector) form – prediction of pressure and velocity to $t^{n+1/2}$ $\rightarrow$ second order of accuracy.

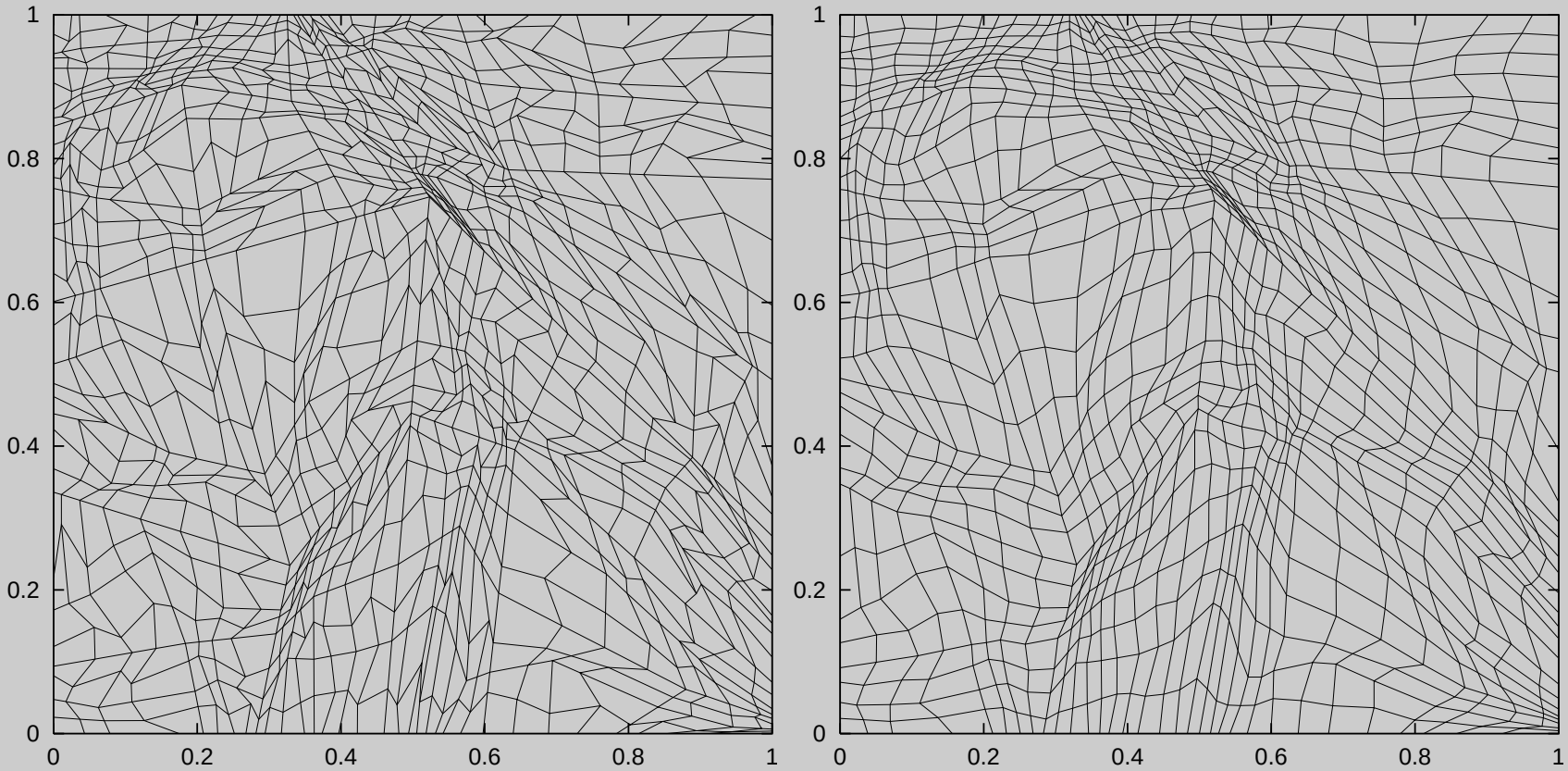
- Next to pressure forces, other forces can be added:
  - Viscosity forces $\vec{F}^q_{c,n}$ – stabilization of the scheme (elimination of oscillations) at shocks, several models[1,2].
  - Subzonal-pressure forces $\vec{F}^{dp}_{c,n}$ – finer pressure discretization, reducing unwanted mesh degeneracies (hourglass)[3].
  - Other forces due to physical modes, such as gravity forces, . . .

[1] Caramana, Shashkov, Whalen: JCP, 1998.
[2] Campbell, Shashkov: JCP, 2001.
[3] Caramana, Shashkov: JCP, 1998.

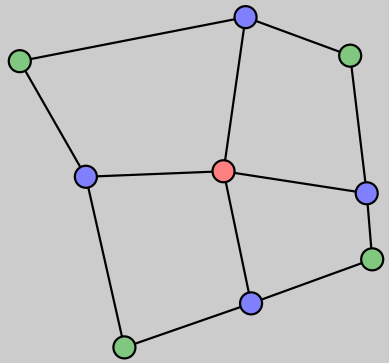
Step 2: Mesh rezoning

- Mesh rezoning = mesh untangling (making it valid) and smoothing (increasing its geometric quality).

- To avoid excessive diffusion of the solution in the following remapping step – move only nodes needed to move, and as little as possible.



Step 2: Mesh rezoning



- Many rezoning methods.
- In realistic computations – efficient methods (3D), e.g. Laplace or Winslow.
- Laplace: new positions as weighted average,

$$\tilde{\vec{x}}_{i,j} = \sum_{k,l=-1,1} w_{i+k,j+l}\, \vec{x}_{i+k,j+l}\,, \text{ where } \sum_{k,l=-1,1} w_{i+k,j+l} = 1\,. \tag{23}$$

- Winslow[1]: based on solving of elliptic PDEs in logical directions,

$$\begin{aligned}\tilde{\vec{x}}_{i,j} \;=\; & \frac{1}{2\left(\alpha^k+\gamma^k\right)}\Big(\alpha^k\left(\vec{x}_{i,j+1}+\vec{x}_{i,j-1}\right)+\gamma^k\left(\vec{x}_{i+1,j}+\vec{x}_{i-1,j}\right) \\ & -\frac{1}{2}\beta^k\left(\vec{x}_{i+1,j+1}-\vec{x}_{i-1,j+1}+\vec{x}_{i-1,j-1}-\vec{x}_{i+1,j-1}\right)\Big),\end{aligned} \tag{24}$$

  where coefficients $\alpha = x_\xi^2 + y_\xi^2$, $\beta = x_\xi\, x_\eta + y_\xi\, y_\eta$, $\gamma = x_\eta^2 + y_\eta^2$, and where (ξ, η) are the logical coordinates.
- More advanced methods – eg. CN minimization, RJM[2]. For untangling – modified CN minimization, feasible set[3].

[1] Winslow: LLNL Report, 1963.
[2] Knupp, Margolin, Shashkov: JCP, 2002.
[3] Berndt, Kucharik, Shashkov: PCS, 2010.

Step 3: Quantity remapping

- Remap = conservative interpolation of all fluid quantities from old (Lagrangian) computational mesh to new (rezoned) one.

- Given: values of given quantity (e.g. density ρ_c) in the cell centroid $\vec{x}_c = \frac{1}{V_c} \int_c \vec{x}\, dV$, $V_c = \int_c 1\, dV$.

- Understood as mean values of unknown underlying density function $\rho(\vec{x})$:

$$m_c = \int_c \rho(\vec{x})\, dV\,, \qquad \rho_c = m_c / V_c\,. \tag{25}$$

- Goal: compute new masses

$$m_{\tilde{c}} \approx \int_{\tilde{c}} \rho(\vec{x})\, dV \tag{26}$$

and mean values $\rho_{\tilde{c}} = m_{\tilde{c}} / V_{\tilde{c}}$ in the rezoned cells $\tilde{c}$.

Step 3: Quantity remapping

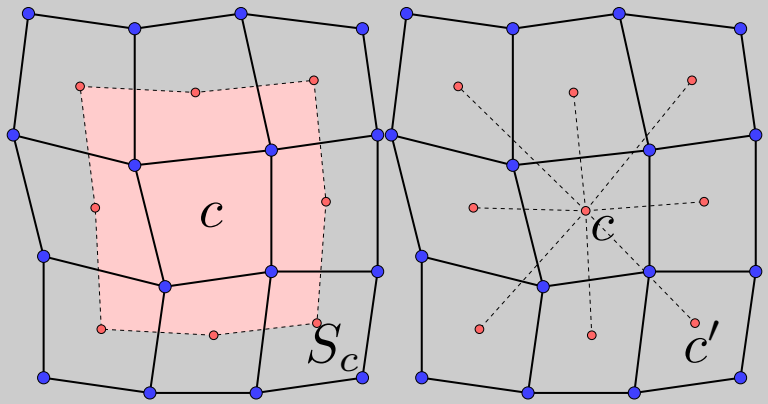
- Requirements:
  - Conservation: $\sum_c m_c = \sum_{\tilde{c}} m_{\tilde{c}}$.
    Solving conservation laws, do not want to spoil it.
  - Accuracy: $\rho_{\tilde{c}} \approx \rho(\tilde{c})$.
    Mean value should be close to the function value in the cell centroid.
  - Linearity-preservation: $\rho(\vec{x})$ linear $\Rightarrow \rho_{\tilde{c}} = \rho(\vec{x}_{\tilde{c}})$.
    Implies second order of convergence.
  - Consistency (continuity): $c = \tilde{c} \Rightarrow \rho_c = \rho_{\tilde{c}}$.
    Do not want to change value is cell did not change.
  - Bound-preservation: $\rho_c^{\min} \leq \rho_{\tilde{c}} \leq \rho_c^{\max}$, where $\rho_c^{\min} = \min_{c' \in C(c)} \rho_{c'}$.
    Only interpolation $\Rightarrow$ do not want to create new extrema.

Step 3: Quantity remapping – Reconstruction

- First phase – piece-wise linear reconstruction of density function (2D):

$$\rho(x,y)\big|_c \approx \rho_c(x,y) = \rho_c + \left(\frac{\partial \rho}{\partial x}\right)_c (x - x_c) + \left(\frac{\partial \rho}{\partial y}\right)_c (y - y_c)\,. \qquad (27)$$

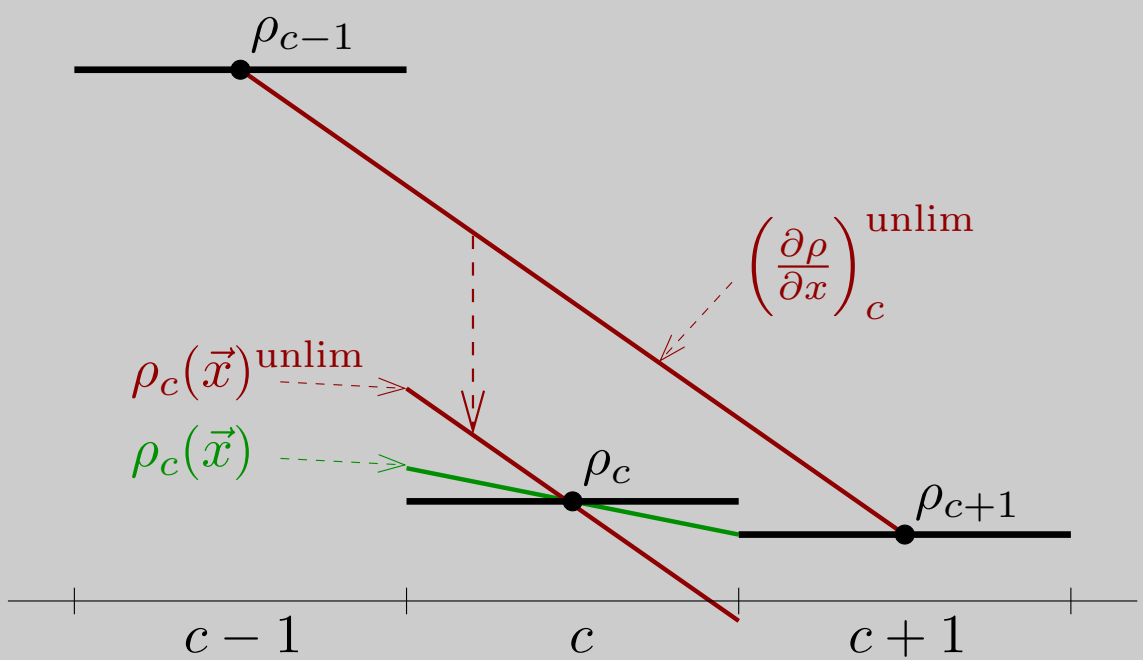
- Slopes $(\partial\rho/\partial x)_c$, $(\partial\rho/\partial y)_c$:
  - Integral average over super-cell: $(\partial\rho/\partial x)_c \approx \frac{1}{V_{S_c}} \int_{S_c} (\partial\rho/\partial x)\, dV$.
  - Minimization (LS) of error functional: $(\partial\rho/\partial x)_c \approx \arg\min \Phi(\partial\rho/\partial x, \partial\rho/\partial x)$, $\Phi(\partial\rho/\partial x, \partial\rho/\partial x) = \sum_{c' \in C(c)} \left\| \rho(\vec{x}_{c'})\big|_c - \rho_{c'} \right\|^2$.
  - Other possibilities.



Step 3: Quantity remapping – Reconstruction

- Usually with limiter, e.g. Barth-Jespersen[1]:
  $(\partial\rho/\partial x)_c = \Psi_c\,(\partial\rho/\partial x)_c^{\mathrm{unlim}}$, where $\Psi_c = \min\limits_{c'\in C(c)} \Psi_{c,n}$, and

$$\Psi_{c,n} = \begin{cases} \min\left(1,\ \frac{\rho_c^{\max}-\rho_c}{\rho_c^{\mathrm{unlim}}(n)-\rho_c}\right) & \text{for } \rho_c^{\mathrm{unlim}}(n)-\rho_c > 0 \\ \min\left(1,\ \frac{\rho_c^{\min}-\rho_c}{\rho_c^{\mathrm{unlim}}(n)-\rho_c}\right) & \text{for } \rho_c^{\mathrm{unlim}}(n)-\rho_c < 0 \\ 1 & \text{for } \rho_c^{\mathrm{unlim}}(n)-\rho_c = 0\,. \end{cases}$$



[1] Barth: Springer, 1997.

Step 3: Quantity remapping – Exact integration

- Most natural method based on cell intersections:
  $m_{\tilde{c}} = \int\limits_{\tilde{c}} \rho(\vec{x})\, dV = \sum\limits_{\forall c'} \int\limits_{\tilde{c}\cap c'} \rho(\vec{x})\, dV \approx \sum\limits_{\forall c'} \int\limits_{\tilde{c}\cap c'} \rho_{c'}(\vec{x})\, dV$.

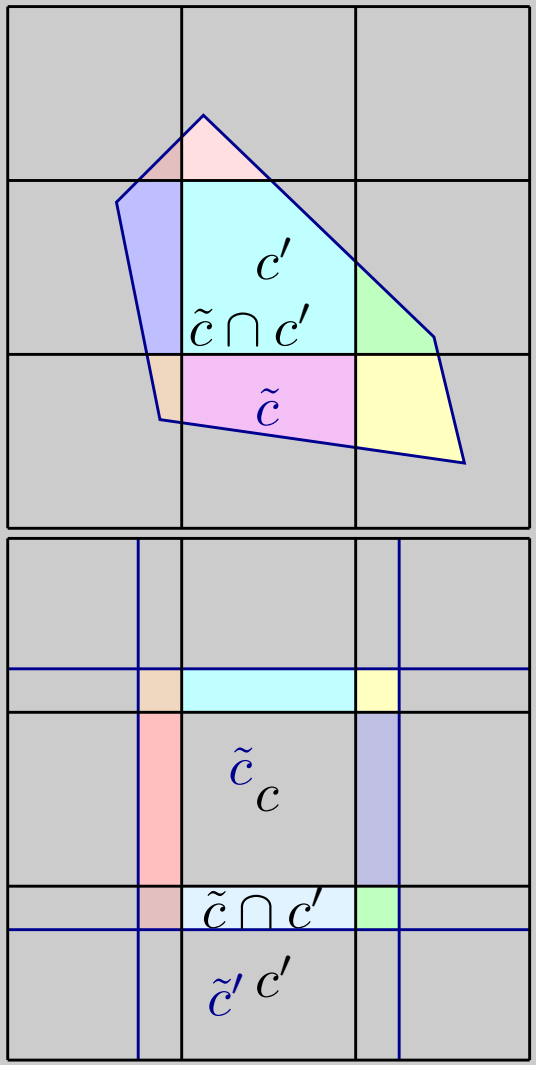
- General geometry $\Rightarrow$ global remap.

- Conservation obvious, limiter $\Rightarrow$ local extrema.

- Same topology $\Rightarrow$ can be formulated in flux form[1]:
  $m_{\tilde{c}} = m_c + \sum\limits_{c' \in C(c)} F^m_{c' \to c}$, $F^m_{c' \to \tilde{c}} = \int\limits_{\tilde{c}\cap c'} \rho_{c'}(\vec{x})\, dV - \int\limits_{\tilde{c}'\cap c} \rho_c(\vec{x})\, dV$.

- Flux form $\Rightarrow$ conservation guaranteed $\Rightarrow$ more freedom in flux construction.

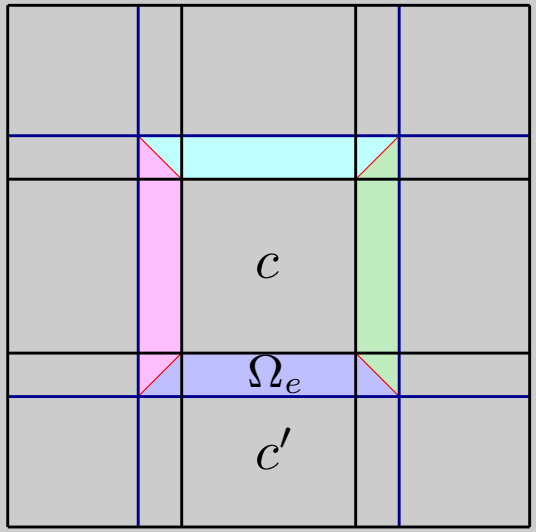
- Problems: computationally expensive, robustness, 3D.



[1] Margolin, Shashkov: JCP, 2003.

Step 3: Quantity remapping – Approximate integration

- Flux approximated using swept regions[1]:
  $m_{\tilde{c}} = m_c + \sum_{e \in \mathcal{E}(c)} F_e^m$, where $F_e^m = \int_{\Omega_e} \rho_{c^*}(\vec{x})\, dV$, $c^* = c/c'$.



- No intersections needed $\Rightarrow$ less computationally expensive, robustness.
- Problem: in certain parts of new cells (corner flux, rotating edge), approximation from wrong cell is used $\Rightarrow$ local bound violation.
- Several options for fixing this:
  - A-posteriori mass redistribution (repair)[2];
  - Flux Corrected Transport (FCT)[3];
  - Multi-dimensional Optimal Order Detection (MOOD)[4];
  - . . .
- Difficult generalization for multi-material case.

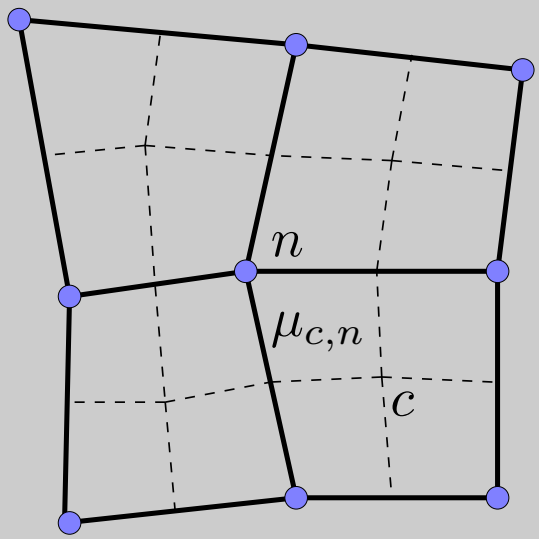
[1] Dukowicz, Baumgardner: JCP, 2000.
[2] Kucharik, Shashkov, Wendroff: JCP, 2003.
[3] Kuzmin, Lohner, Turek: Springer, 2005.
[4] Blanchard, Loubere: C&F, 2016.

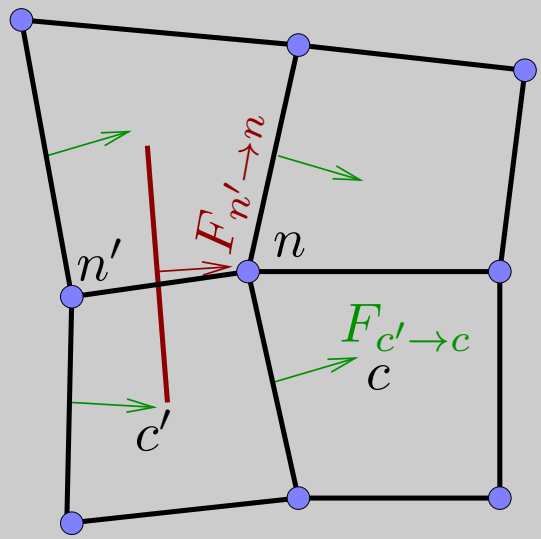
Remap of all fluid quantities

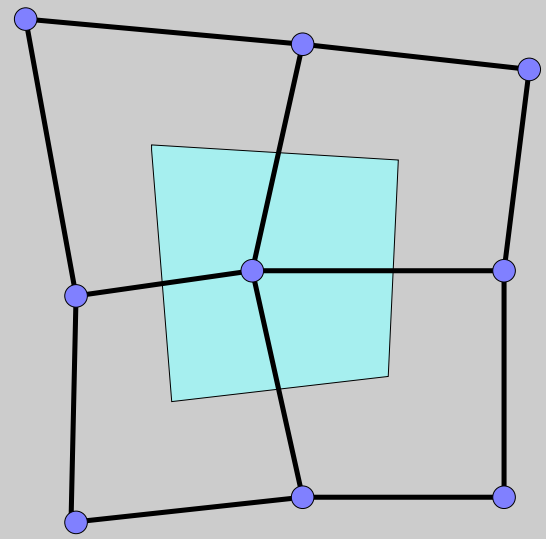
- Up to now – only remap of ρ, m.
- Remap of ε – similar as density.
- Pressure – usually computed from EOS, but can be remapped too.
- Remap of $\vec{w}$ – simple in cell-centered methods (same manner), more complicated in staggered discretization.
- Kinetic energy computed from remapped velocities – non-linear $\rightarrow$ violation of kinetic energy conservation $\Rightarrow$ wrong shock speeds, wrong plateau height, ...
- Typically treated by energy fix[1]: remap kinetic energy independently and distribute its discrepancy to internal energy.
- Several options for velocity remap.

[1] Benson: CMAME, 1992.

Remap of all fluid quantities







- Double-fine mesh[1].
- Simplest way:
  - $\mu_{c,n} = m_{c,n}\, u_n$,
  - remap $\mu_{c,n} \to \mu_{\tilde{c},\tilde{n}}$,
  - $u_{\tilde{n}} = \sum_{c' \in C(n)} \mu_{\tilde{c}',\tilde{n}} / m_{\tilde{n}}$.

- Inter-nodal fluxes[2].
- Interpolation of $F^m_{n'\to n}$ from $\forall\, F^m_{c'\to c}$, μ flux: $F^\mu_{n'\to n} = u^{\mathrm{rec}}_{n'\to n}\, F^m_{n'\to n}$.
- $u_{\tilde{n}} = \dfrac{\mu_n + \sum_{n' \in N(n)} F^\mu_{n'\to n}}{m_{\tilde{n}}}$.

- Remap on dual cells[3].
- The rest same as for other quantities.

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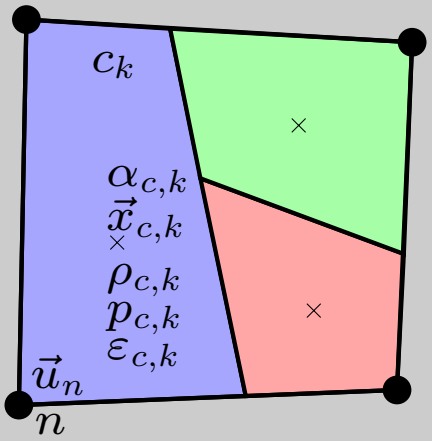
[1] Loubere, Shashkov: JCP, 2005.
[2] Kucharik, Shashkov: JCP, 2014.
[3] Hirt, Amsden: LANL Report, 1973.

Multi-material ALE



- Lagrangian simulation – different materials in different cells, remain there for the whole simulation.
- ALE $\Rightarrow$ mixing unavoidable $\Rightarrow$ numerical interface diffusion, useless EOS, . . .
- Solution: multi-material ALE.
- Concentrations $\times$ splitting of cell c to polygons c_k representing particular materials k, thermodynamic quantities separately for each material.
- Additional: material quantities – relative volume (volume fraction) $\alpha_{c,k}$, eventually approximate material position (centroid) $\vec{x}_{c,k}$.
- Splitting of c to c_k = material reconstruction[1]: Volume of Fluid (VOF)[2], Moment of Fluid (MOF)[3], . . .

[1] Kucharik, Garimella, Schofield, Shashkov: JCP, 2010.
[2] Youngs: AWE Report, 1984.
[3] Dyadechko, Shashkov: JCP, 2008.

Multi-material ALE – Differences

- In Lagrangian step – additional model for material interaction (closure model) defining interface motion $\rightarrow$ evolution of $\alpha_{c,k}$.
- In rezone – no difference. Methods minimizing rezone at material interfaces.
- In remap – generalization of exact integration $\rightarrow$ instead of intersection with original cell c, so intersections with all its material polygons c_k[1].
- Next to remap of standard fluid quantities, remap of $\alpha_{c,k}$ and $\vec{x}_{c,k}$.
- Reconstruction/remap of velocity vector must be performed in a consistent way, otherwise can lead to conservation violation due to non-linearity of kinetic energy[2], or symmetry violation of velocity field[3].

[1] Kucharik, Shashkov: JCP, 2014.
[2] Bailey, Berndt, Kucharik, Shashkov: JCAM, 2010.
[3] Velechovsky, Kucharik, Liska, Shashkov, Vachal: JCP, 2013.

Physical aspects – Model

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

$$\frac{d\,\rho}{d\,t} = -\rho\,\nabla\cdot\vec{w}\,, \tag{28}$$

$$\rho\,\frac{d\,\vec{w}}{d\,t} = -\nabla\,p\,, \tag{29}$$

$$\rho\,\frac{d\,\varepsilon}{d\,t} = -p\,\nabla\cdot\vec{w} + \nabla\cdot(\kappa\nabla T) - \nabla\cdot\vec{I}\,, \tag{30}$$

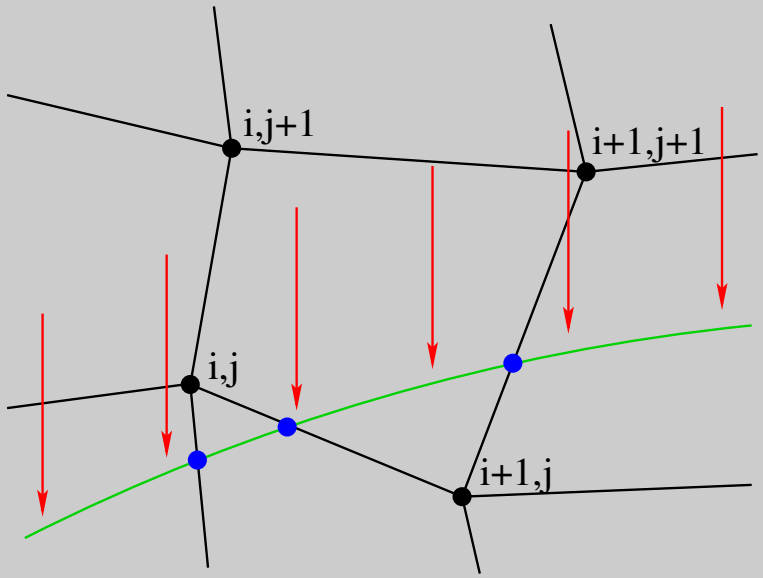
where T is temperature, κ is heat conductivity coefficient, and $\vec{I}$ is laser beam intensity profile.

[1] Kucharik, Shashkov: JCP, 2014.
[2] Bailey, Berndt, Kucharik, Shashkov: JCAM, 2010.
[3] Velechovsky, Kucharik, Liska, Shashkov, Vachal: JCP, 2013.

Physical aspects – Laser absorption

- Simple model of laser absorption on the critical surface[1].
- Laser radiating from upwards – $\vec{I} = (0, -I_z(t,r))$, Gaussian profile.
- On each edge – projection of intensity to the normal direction $\vec{I}_e$.
- Interpolation of nodal density from neighbors.
- Density in all cell nodes sub- or super-critical $\Rightarrow (D\,\vec{I})_c = 0$.
- Mixed $\Rightarrow \quad (D\,\vec{I})_c = \frac{1}{V_c} \sum_{e \in \delta c} L^s(e)\,\vec{I}_e$,

  $L^s(e)$ – subcritical edge length,
  $\vec{I}_e$ – projected intensity along edge.



- Equation of absorption: $\rho\,\frac{d\,\varepsilon}{d\,t} + p\,\nabla \cdot \vec{w} = -C_A\,\nabla \cdot \vec{I}$, C_A – coefficient.

[1] Liska, Kucharik: EQUADIFF, 2007.

Physical aspects – Laser absorption

- Problems – C_A needed from user + full absorption in one cell leading to series of "cell explosions".
- Several more advanced models.
- Raytracing[1] – 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[2].

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

Physical aspects – Heat conductivity

- Represented by parabolic term in the energy equation.
- Separated by operator splitting to the form $\rho\,\varepsilon_t = \nabla\cdot(\kappa\,\nabla T)$, transformed to temperatures $T_t = \frac{1}{\rho\,\varepsilon_T}\nabla\cdot(\kappa\,\nabla T)$.
- Solving using support operators method[1].
- Temperature derivative of energy ε_T computed numerically.
- Classical Spitzer-Harm heat conductivity coefficient

$$\kappa = 20\left(\frac{2}{\pi}\right)^{3/2}\frac{k^{7/2}}{\sqrt{m_e}\,e^4}\,\delta_{ee}\,\frac{T^{5/2}}{Z\,\ln\Lambda} \tag{31}$$

corrected by electron-electron collision term $\delta_{ee} = 0.095\,\frac{Z+0.24}{1+0.24\,Z}$, where k is Boltzmann constant, m_e is the electron mass unit, e is the electron charge, Z is the plasma mean ion charge, and $\ln\Lambda$ is the Coulomb logarithm.

[1] Shashkov, Steinberg: JCP, 1996.

Physical aspects – Heat conductivity

- Green/Gauss theorems express integral properties of operators:
  - Generalized gradient $\vec{W} = \vec{G}T = -\kappa \nabla T$
  - Extended divergence $\vec{D}\,\vec{W} = \left[\begin{array}{lll} \nabla \vec{W} & \text{in} & V \\ -(\vec{W}, \vec{n}) & \text{on} & \partial V \end{array} \right.$
- Mimetic discrete operators G, D have the same discrete integral properties, namely gradient is adjoint of divergence $G = D^*$.
- Fully implicit scheme in time $(T^{n+1} - T^n)/\Delta t + D\,G\,T^{n+1} = 0$.
- Explicit not suitable: CFL $\Rightarrow$ many steps per 1 Lagrangian step.
- Matrix of global system is symmetric and positive definite – conjugate gradient method.
- Exact on piecewise linear solutions, otherwise it is second order accurate in space. Works well on bad quality meshes, allows discontinuous diffusion coefficient.

Physical aspects – Heat flux limiter

- Standard methods can provide higher heat flux $\vec{W}$ than physically feasible – need to limit it.

- Compare sizes of heat fluxes with local free stream limit $W^{lim} = f^{\max} \frac{k}{m_u} \sqrt{\frac{k}{m_e}} \frac{Z\,\rho}{A} T^{3/2}$, where the coefficient $f^{\max} \in (0.05, 0.3)$ (between 5% and 30% of the physical limit).

- Compute values $c = \frac{W^{lim}}{|\vec{W}|}$, and renormalize the conductivity coefficient $\tilde{\kappa} = c\,\kappa$ in each cell.

- The conductivity equation is then solved for the second time with new $\tilde{\kappa}$, ensuring the limit is not exceeded.

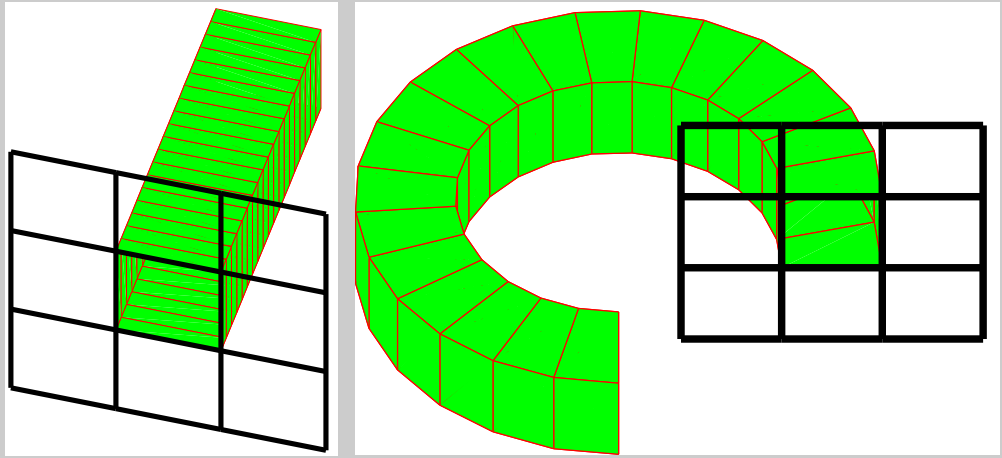
- Need to solve the global system twice $\rightarrow$ new temperatures/energies more realistic.

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

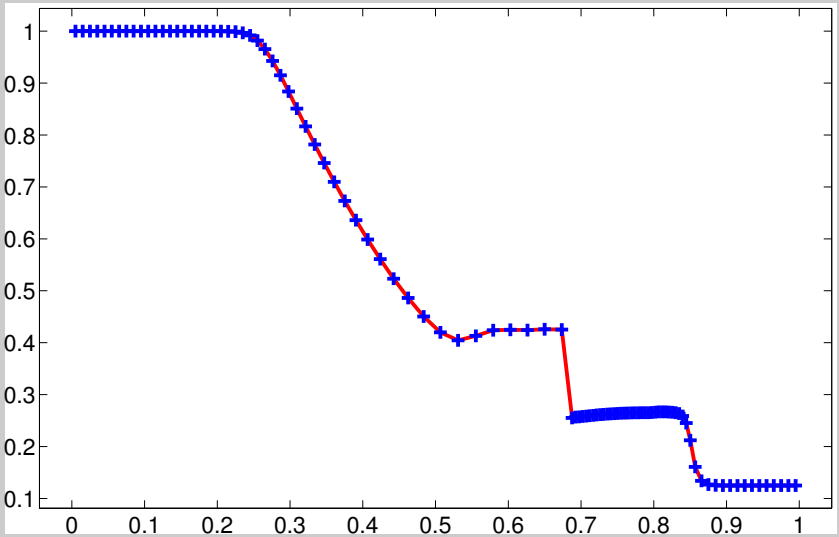


- Many laser-related processes are cylindrically symmetrical, 2D code with cylindrical geometry well approximates 3D reality.
- Switching to cylindrical geometry = adding r factor into all integrals – different volumes, centroids.
- Lagrangian solver – adding r factor leads to Control Volume scheme: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

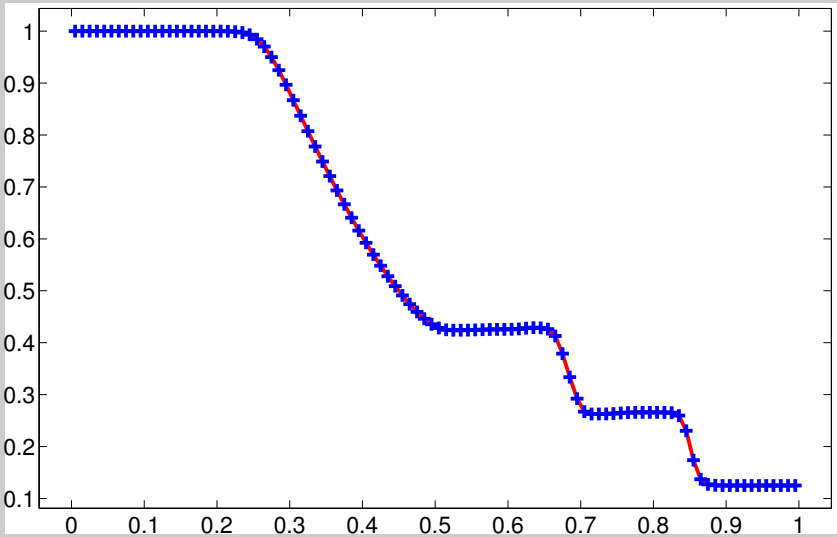
Physical aspects – Others

- 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.
- Most of described methods implemented in Prague ALE (PALE) code – Fortran, 2D Cartesian/cylindrical geometry, staggered ALE, realistic EOSes, laser absorption, heat conductivity + limiter, two-temperature model, . . .
- Simulations of laser/target interactions, experiments at PALS or ELI.

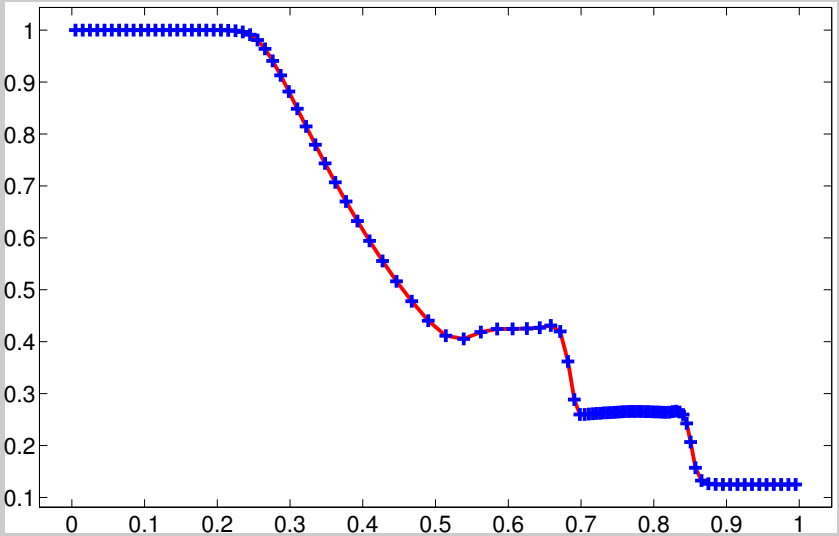
Fluid examples: 1D Sod problem



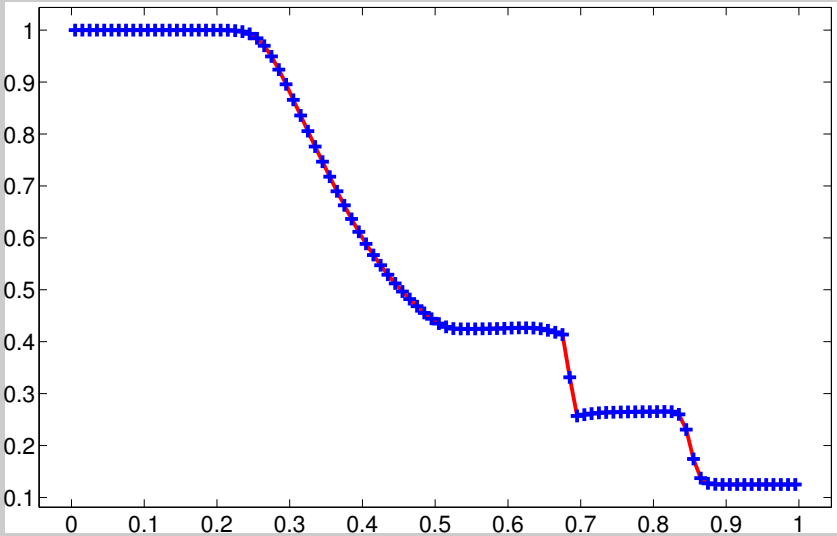
Lagrangian



Eulerian



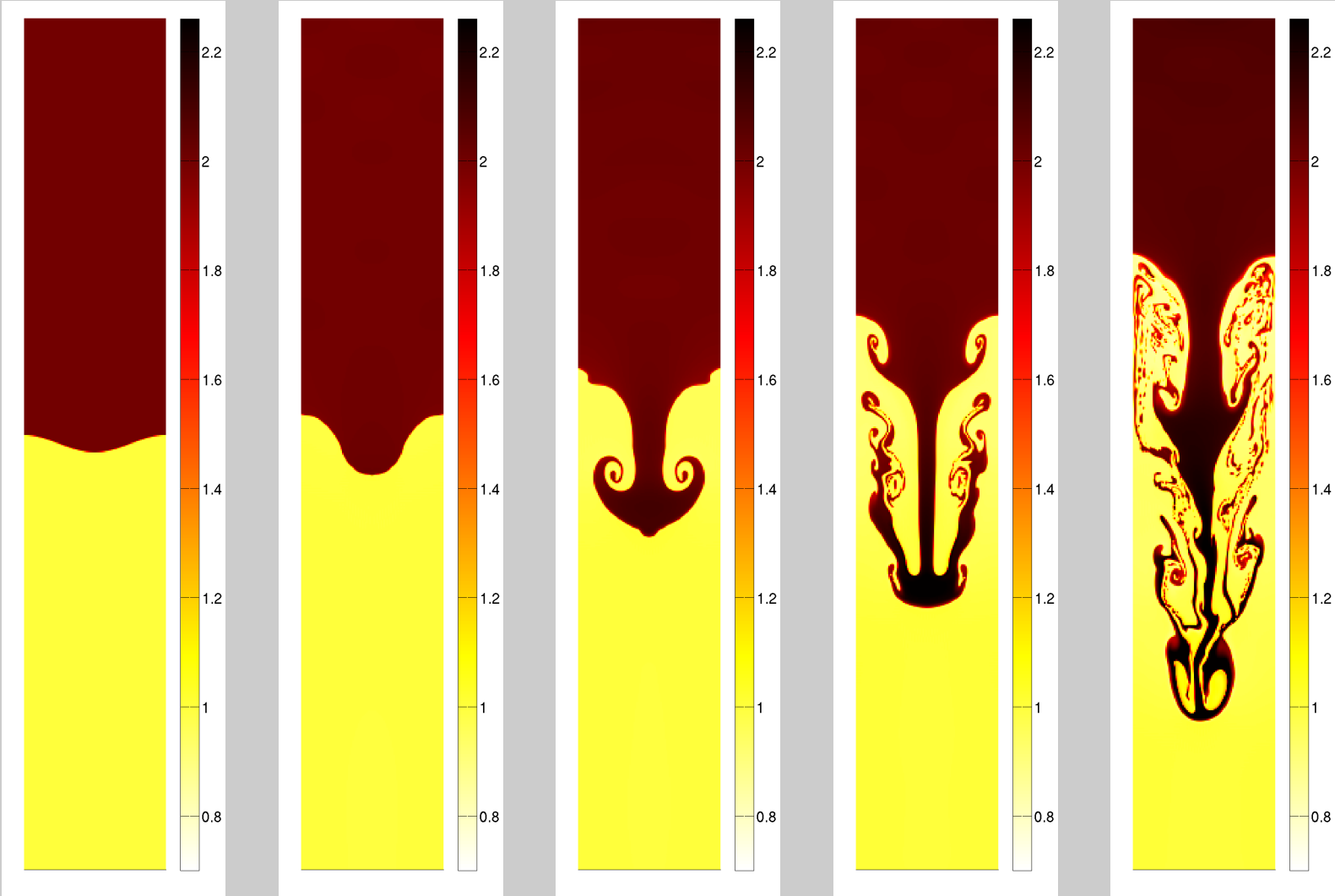
ALE 10



MM Eulerian

Fluid examples: Rayleigh-Taylor instability

100×600 mesh, MM, Eulerian regime[1].



$T = 0$ $T = 5$ $T = 10$ $T = 15$ $T = 20$

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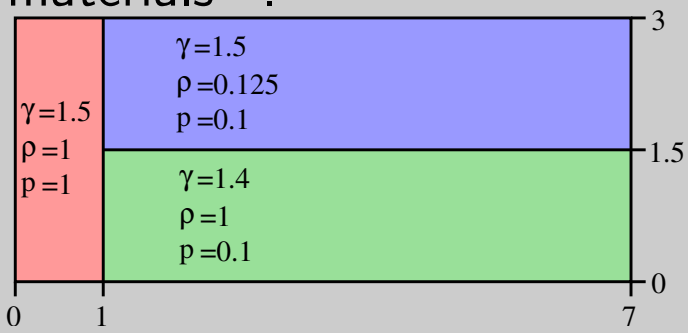
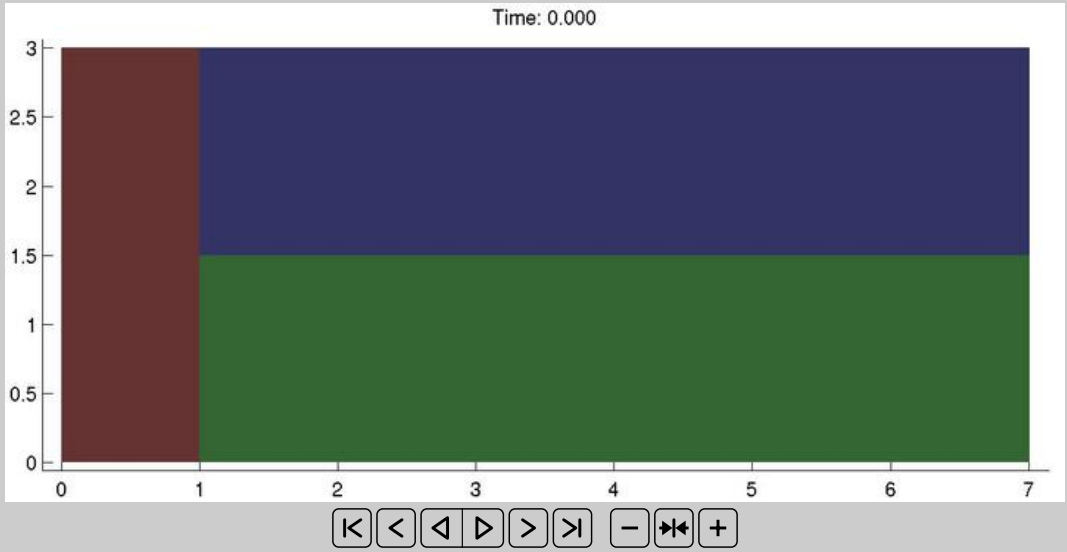
[1] Fung, Francois, Dendy, Kenamond, Lowrie: NECDC, 2006.

Fluid examples: Triple point problem

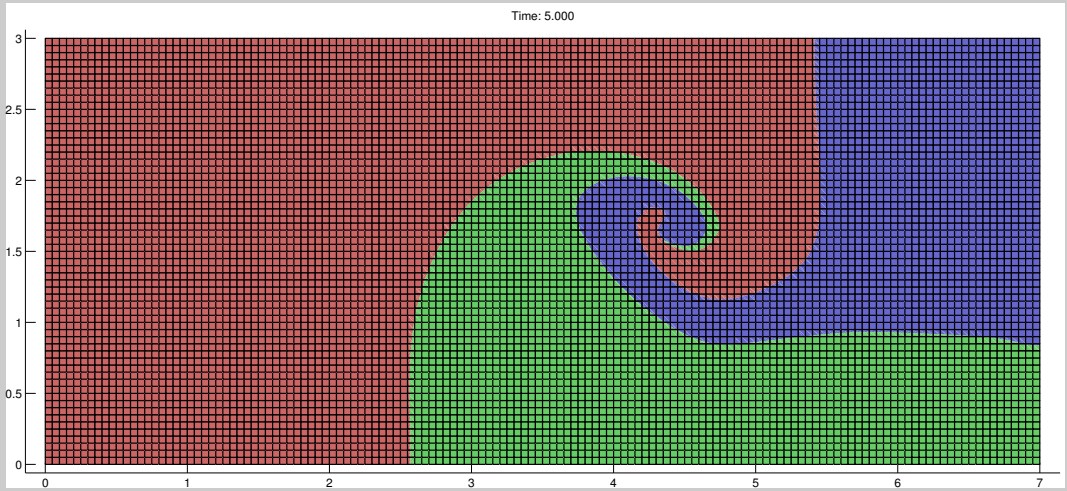
- Interfaces among three materials[1].





- Higher pressure generates shock, different properties of right materials ⇒ vortex.

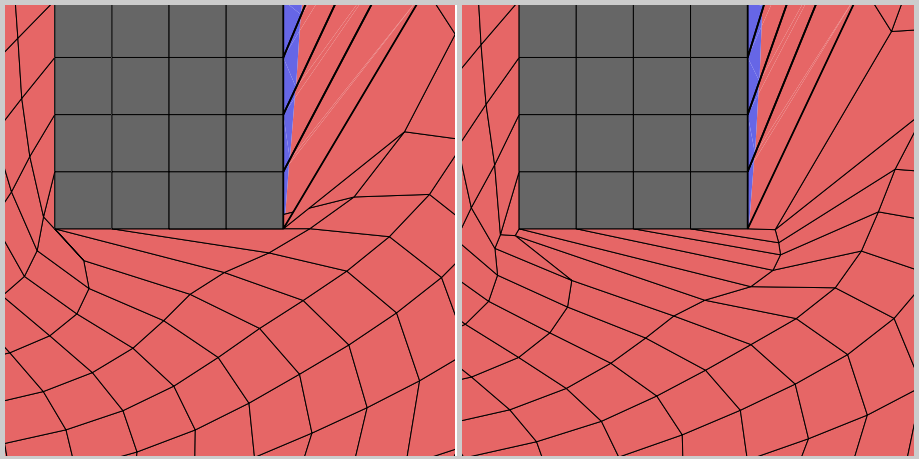
- Eulerian run, thin filaments.

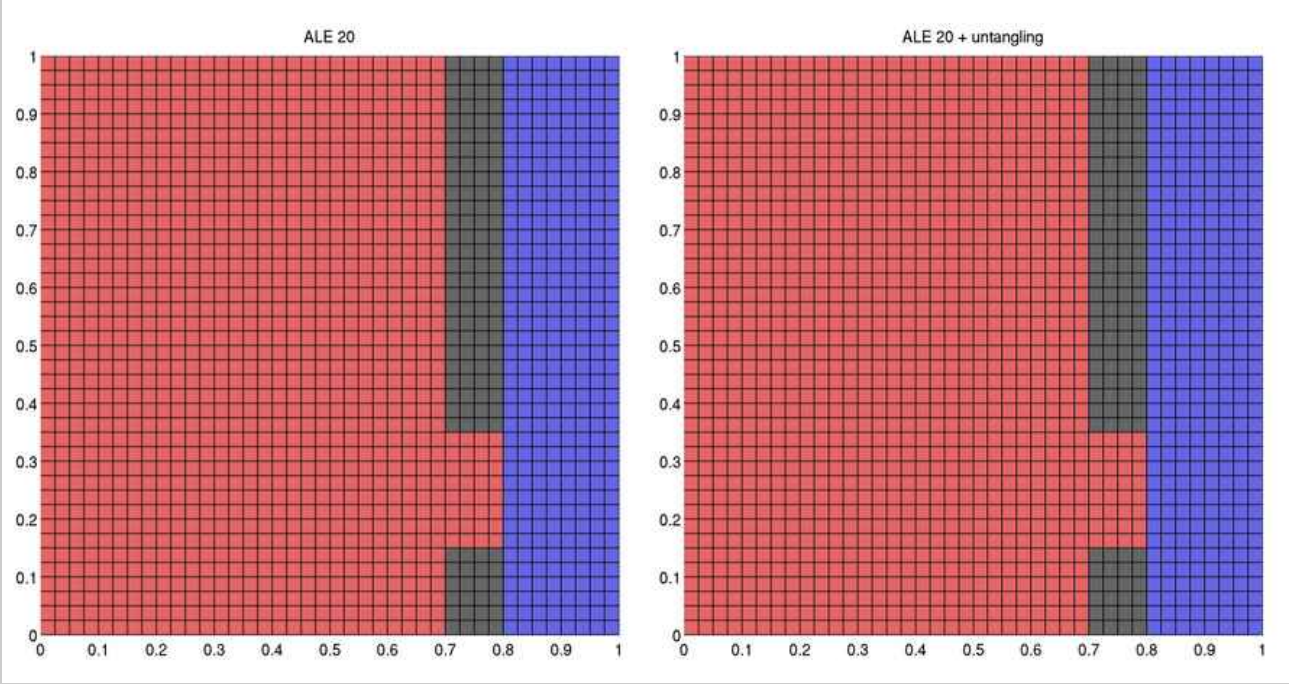


[1] Galera, Maire, Breil: JCP, 2010.

Fluid examples: Jet through a hole in a wall

- Hole in a wall[1] (inactive cells), larger left pressure ⇒ jet.
- Deformation of cells around the hole, ALE simulation failure.
- Feasible-set mesh untangling ⇒ increased robustness.

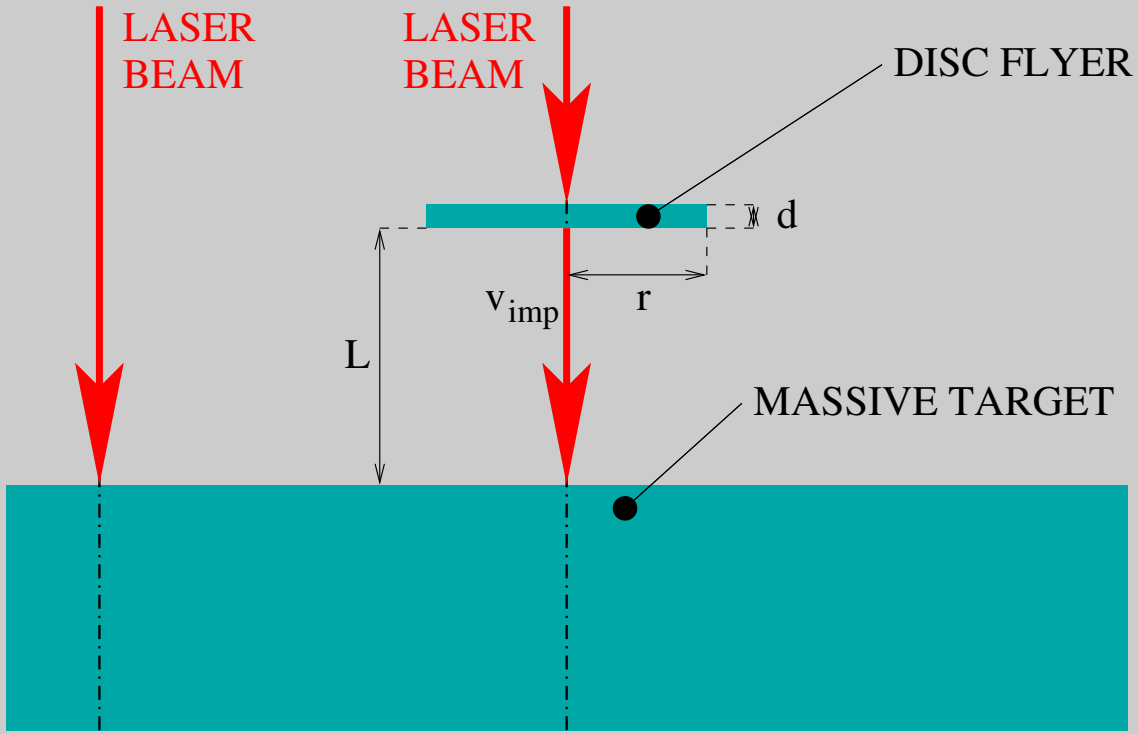




[1] Berndt, Kucharik, Shashkov: PCS, 2010.

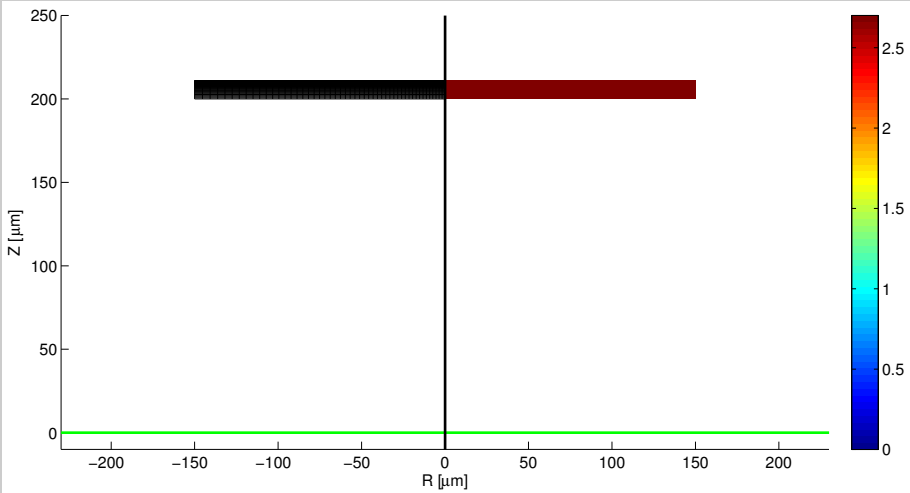
Laser examples: Disc impact

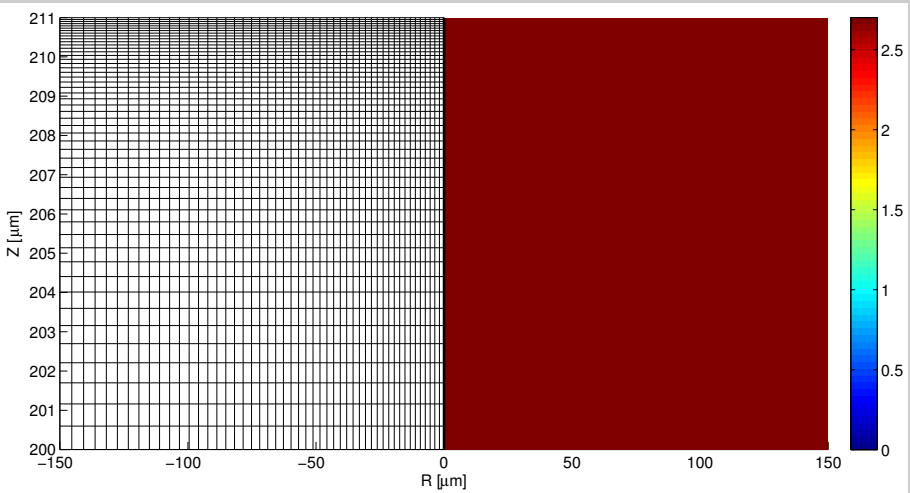
- Simulation inspired by experiments on PALS system[1].
- Laser evaporates disc target, acceleration to tens/hundreds km/s[2].
- Impact to massive target.
- Melting and evaporation of material, crater formation.



[1] Borodziuk, Kasperczuk, Pisarczyk, et al.: CzJP, 2003.
[2] Kalal, Borodziuk, Demchenko, et al.: ECLIM, 2004.

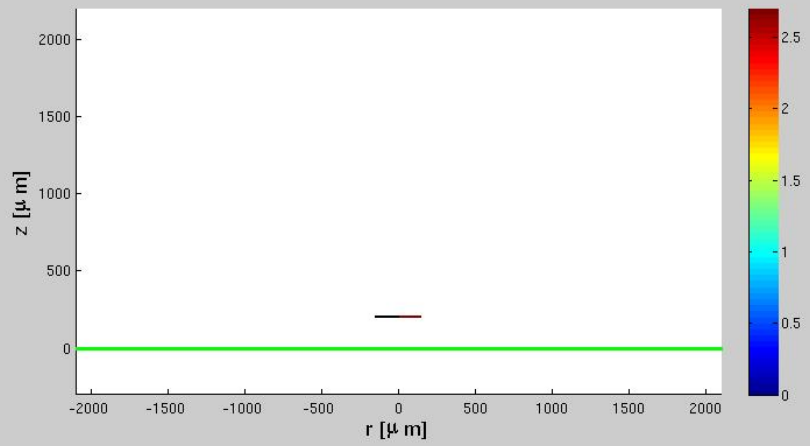
Laser examples: Disc impact – 1) ablative acceleration

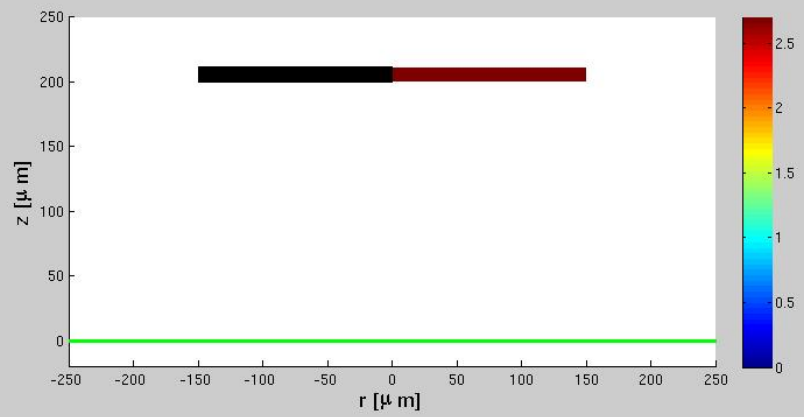


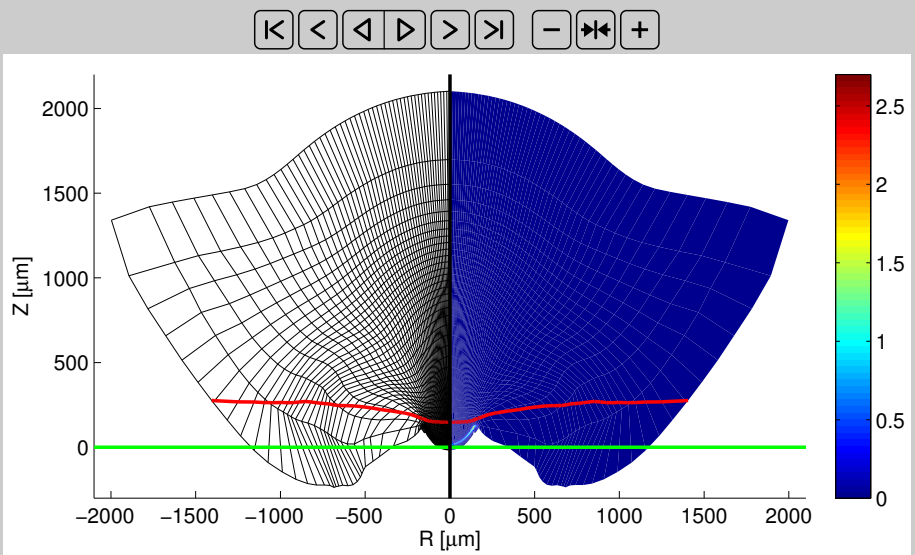


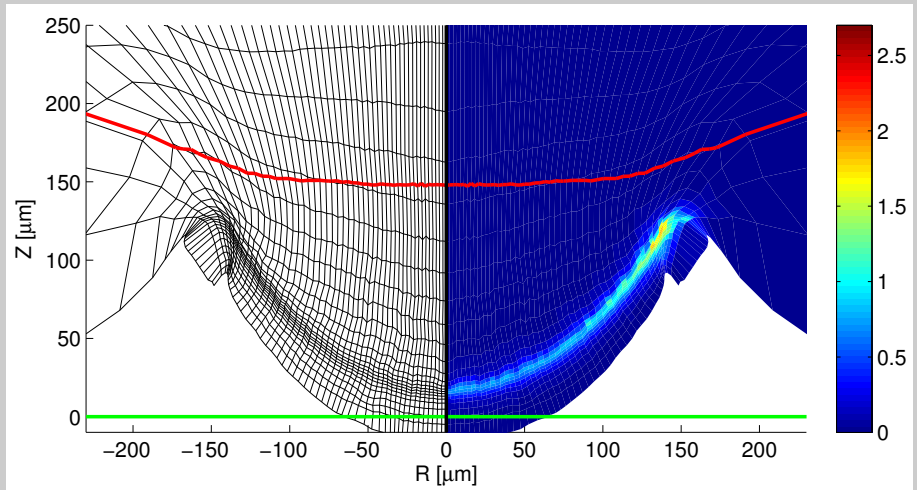
- Geometrical computational mesh, in disc only.
- Laser absorption, material evaporation upwards.
- Massive part of the disc accelerated downward due to ablation (momentum conservation).

Laser examples: Disc impact – 1) ablative acceleration

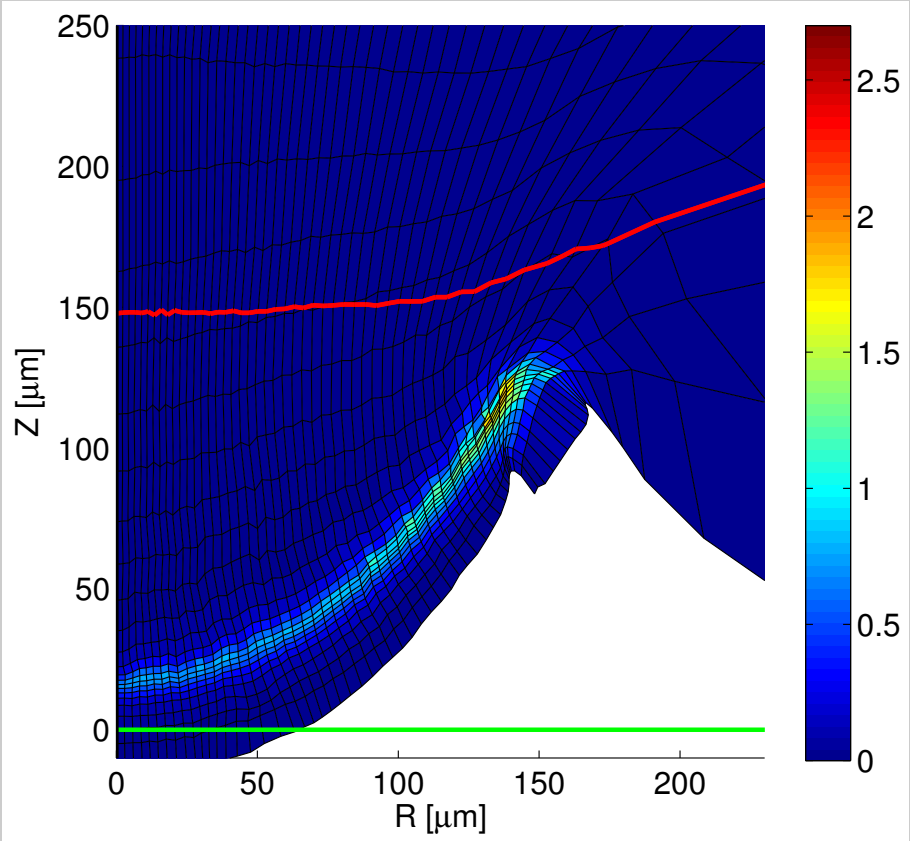


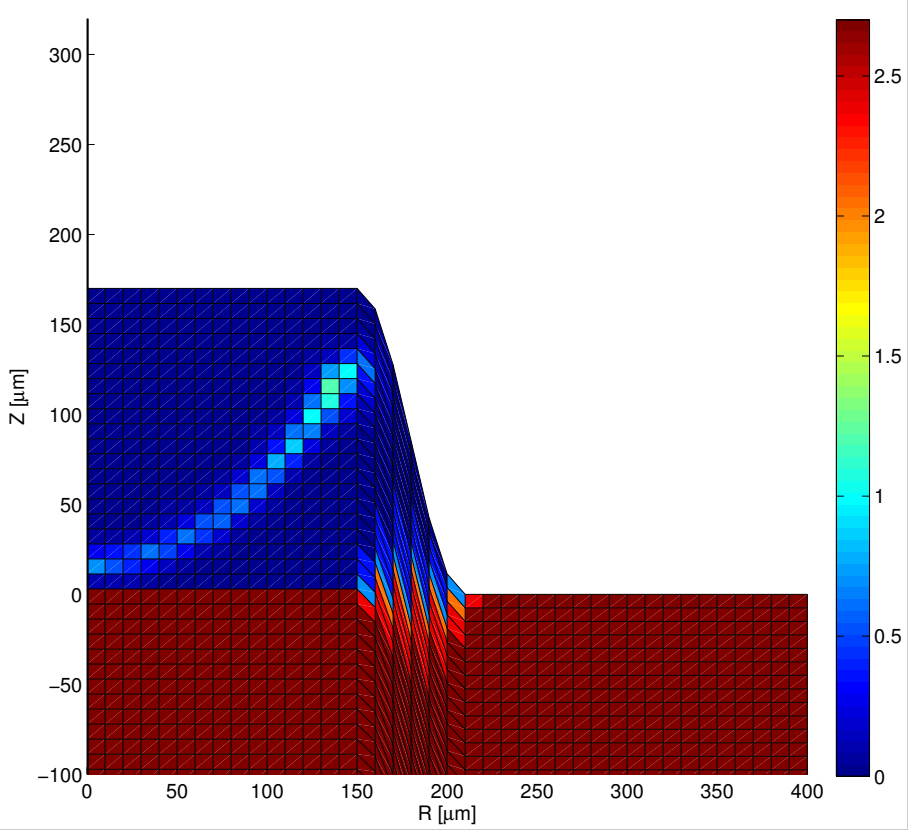




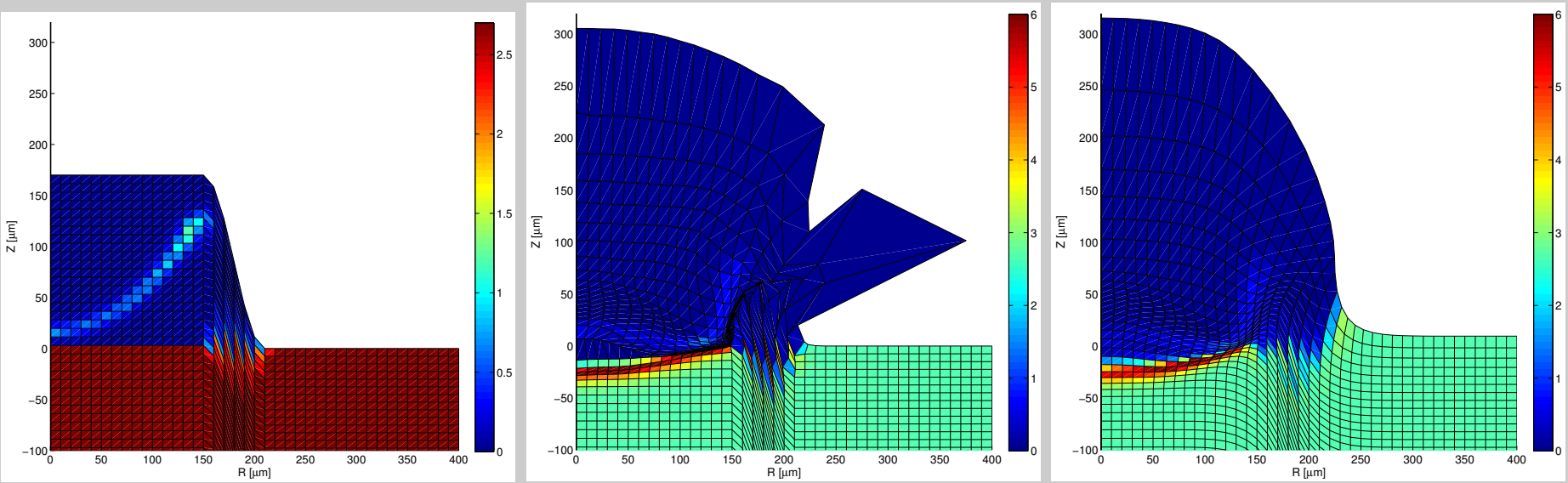


Laser examples: Disc impact – 2) interpolation





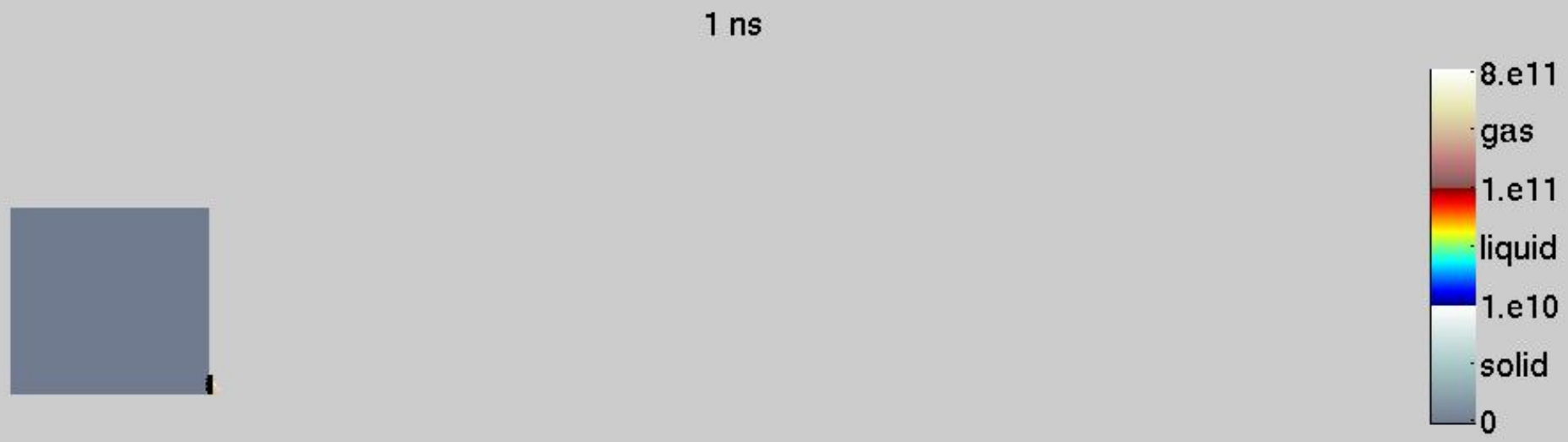
Laser examples: Disc impact – 3) impact, crater



- Comparison of Lagrangian and ALE simulation short after computation starts, Lagrangian fails.
- ALE does not influence the result too much (slight shock diffusion), but mesh improved significantly.
- Impossible to finish simulation without ALE.

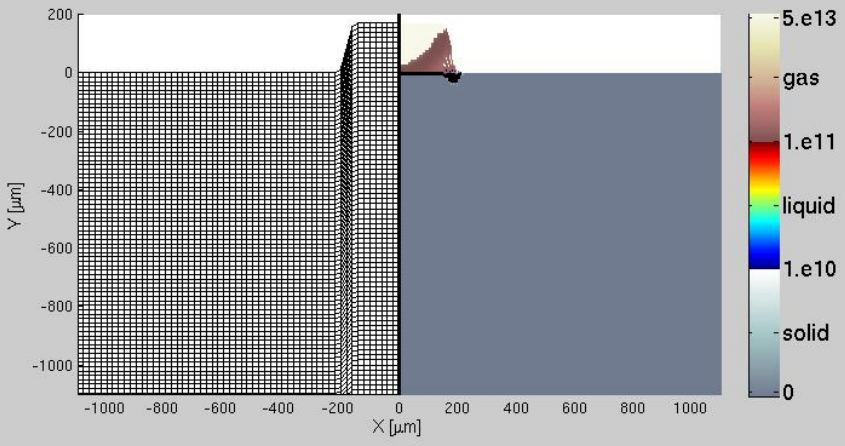
Laser examples: Disc impact – 3) impact, crater

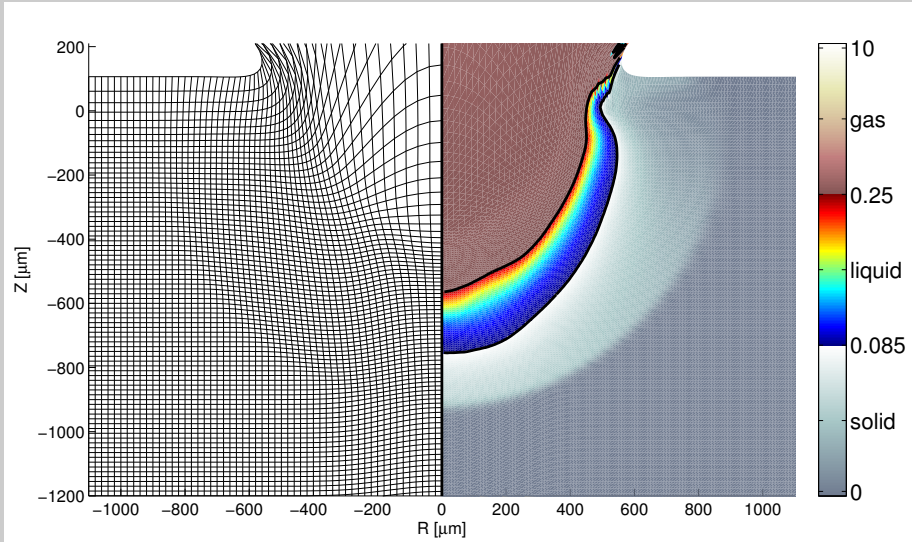
- After impact – material compression, increase of temperature.
- Inside target: circular shock wave spreading from impact, melting and evaporation of target.
- Corona (plasma plume) spreading outside.



Laser examples: Disc impact – 3) impact, crater

- Crater formation – liquid/gas phase interface.
- Mesh remains smooth, the simulation can continue further.
- Comparison of crates sizes to experimental values – reasonable agreement[1]

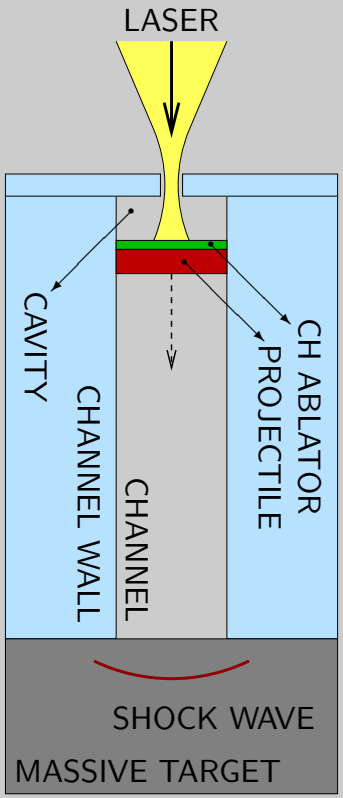




[1] Kucharik, Limpouch, Liska, Havlik: ECLIM, 2004.

Laser examples: LICPA scheme

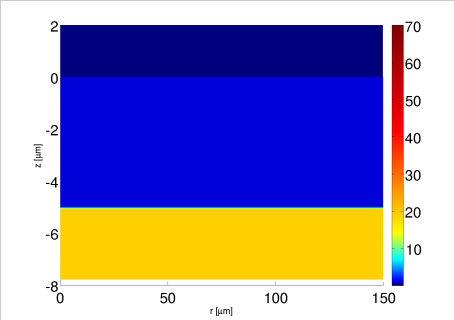
- Laser induced cavity pressure acceleration[1].
- Preparation, analysis, interpretation of PALS experiments.
- Simulations of processes in channel covered by a cavity.
- Cavity ⇒ large portion of laser energy transferred to shock wave ⇒ higher impact velocity, larger craters.
- Many configurations: with 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.



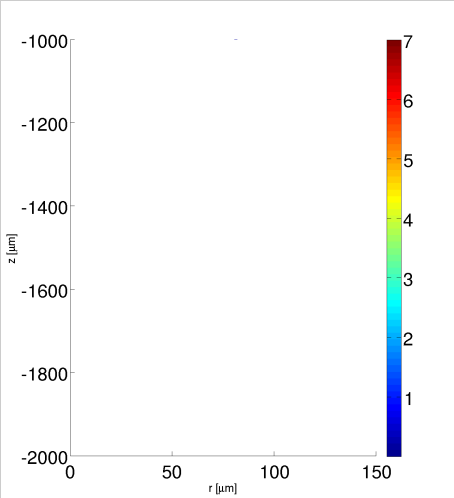
[1] Badziak, Borodziuk, Pisarczyk, et al.: APL, 2010.

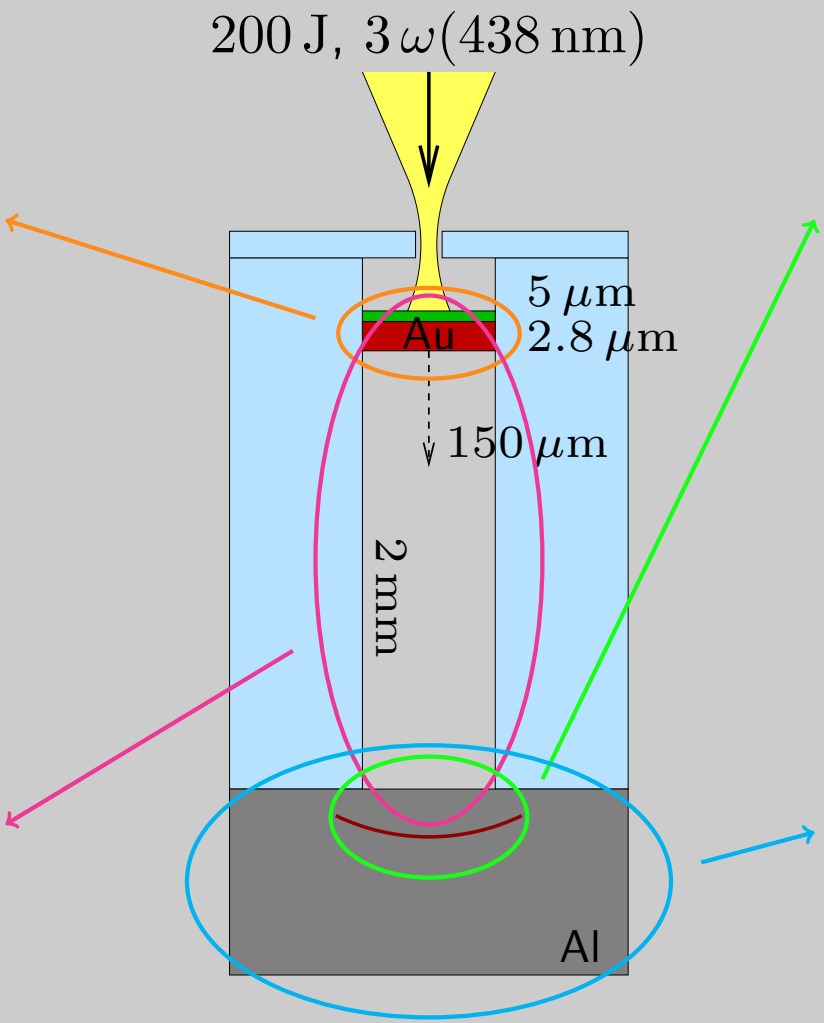
Laser examples: LICPA scheme

Absorption

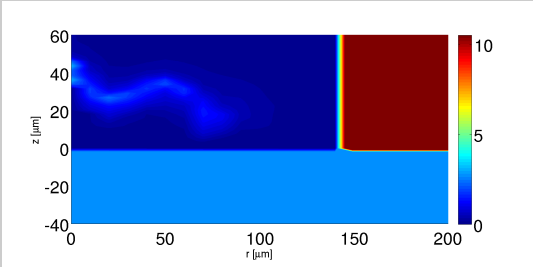


Accel. + impact

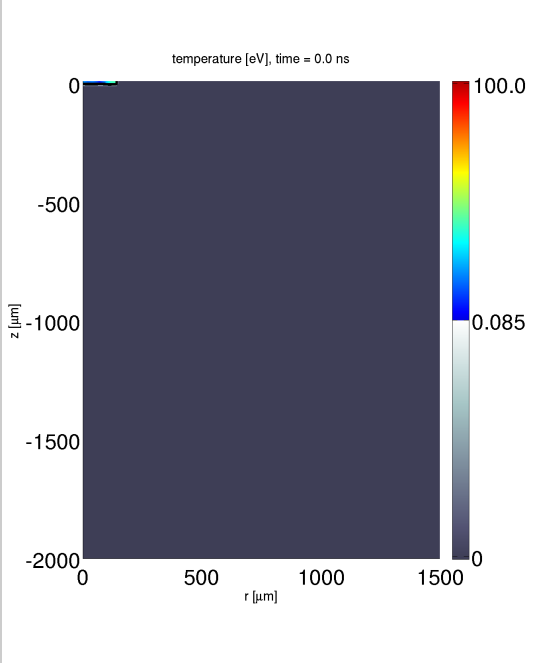




Shock formation



Crater development



New trends in ALE hydrodynamics

- ALE+AMR (Adaptive Mesh Refinement)[1]
  - automatically finer mesh in interesting regions (shocks, interfaces, physical phenomena, . . .);
  - higher effective resolution, uncomputable in whole domain;
  - necessary in Eulerian codes, useful in ALE.

- ReALE – reconnection ALE[2]
  - changing mesh topology, cell follows the fluid;
  - significant improvement in regions of sheer flows or vortices.

- Curvilinear ALE[3] – curved mesh instead of straight
  - cell can significantly deform during fluid motion;
  - prevents most of tangling, increased robustness, less ALE.

[1] Anderson, Elliott, Pember: JCP, 2004.
[2] Loubere, Maire, Shashkov, Breil, Galera: JCP, 2010.
[3] Anderson, Dobrev, Kolev, Rieben, Tomov: SIAM JSC, 2018.

Conclusions

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

Thank you for your attention.