Milan Kucharík; Richard Liska; Pavel Váchal; Mikhail Shashkov

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ARBITRARY LAGRANGIAN-EULERIAN (ALE) METHODS IN COMPRESSIBLE FLUID DYNAMICS*

Milan Kuchařík, Richard Liska, Pavel Váchal, Mikhail Shashkov

Abstract

The aim of this paper is to present an Arbitrary Lagrangian-Eulerian (ALE [1]) code for simulation of problems in compressible fluid dynamics and plasma physics including heat conduction and laser absorption, in both Cartesian and cylindrical geometries. Various techniques are utilized for mesh adaptation (rezoning), including Winslow smoothing [2], three-step untangling [3] and Reference Jacobian method [4, 5]. For conservative transfer (remapping) of variables onto the rezoned mesh, linear interpolation with a posteriori repairs is used by default. Simulation of high velocity impact, for which pure Lagrangian method fails, proves the usefulness of ALE approach.

1. Introduction

The Arbitrary Lagrangian-Eulerian (ALE) method [1] is a popular tool for simulation of continuum mechanics problems with large shear deformation such as fluid flow and metal forming. Compared to pure Eulerian methods, it is also better suited for moving boundaries and large volume changes of the computational domain, appearing in simulations of laser-plasma interactions and inertial confinement fusion.

The ALE algorithm consists of a classical Lagrangian step in which the mesh moves along with the modeled material, a rezone step in which the mesh is modified to preserve good quality through the computation, and a remapping step in which the solution is conservatively transferred from the old mesh to the new, rezoned one. We present new efficient techniques for the rezoning and remapping stages of the ALE framework and demonstrate some of their properties on a real physical simulation of high velocity impact.

Note that by the ALE method we understand the variation of Lagrangian hydrodynamics which avoids Lagrangian mesh distortion (arising in some problems involving e.g. shear flows) by rezoning and remapping. Another method, unfortunately also called ALE, uses a mesh smoothly moving in a predefined way, typically determined by moving boundaries rather than by fluid motion.

Details on implementation of particular procedures and on the physical background can be found in [6].

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2. The Lagrangian step

In pure Lagrangian computation, each mesh cell can be considered as a particle of the fluid, so that the mesh moves along with the simulated problem, with no mass flux between the cells. Euler equations for compressible fluid flow with heat conductivity and laser absorption in Lagrangian coordinates read

$$\frac{1}{\rho}\frac{\mathrm{d}\,\rho}{\mathrm{d}\,t} = -\nabla\cdot\vec{v}, \qquad \rho\frac{\mathrm{d}\,\vec{v}}{\mathrm{d}\,t} = -\nabla p, \qquad \frac{\mathrm{d}\,\vec{x}}{\mathrm{d}\,t} = \vec{v}, \tag{1a}$$

$$\rho\,\frac{\mathrm{d}\,\varepsilon}{\mathrm{d}\,t} = -p\,\nabla\cdot\vec{v} + \nabla\cdot(\kappa\nabla T) - C_a\nabla\cdot\vec{I}, \tag{1b}$$

where total Lagrangian time derivatives include convective terms: $\frac{\mathrm{d}}{\mathrm{d}\,t} = \frac{\partial}{\partial t} + \vec{v}\cdot\nabla$. Scalar quantities (density ρ, pressure p, specific internal energy ε and temperature T) are approximated in mesh cells, while vectors (position $\vec{x}$ and velocity $\vec{v}$) are related to the nodes. To complete the system, one has to supply also the equation of state (EOS). For the ideal polytropic gas, the EOS is $p = (\gamma - 1)\varepsilon\rho$. For other materials, more sophisticated formulas are advised, e.g. the Quotidian EOS [7]. The hyperbolic Lagrangian system is numerically treated by compatible method [8, 9] conserving total energy. Several types of artificial viscosity are incorporated into the difference scheme, such as bulk viscosity, edge viscosity, etc. [6]. Laser absorption is taken into account by the last term in the energy equation (1b).

The system is split into hyperbolic and parabolic parts. The parabolic part

$$\frac{\mathrm{d}\,T}{\mathrm{d}\,t} - \nabla\cdot(\kappa\nabla T) = 0$$

of the energy equation is solved separately by a scheme fully implicit in time, which allows the choice of timestep equal to that of the hyperbolic system. A discretization of operators div and grad by a mimetic method [10] leads to a system with a symmetric and positive definite matrix, which is then solved by conjugate gradient method.

3. Mesh adaptation (rezoning)

During the rezoning process, the quality of strongly deformed parts of the mesh must be improved, so that the computation can continue with desired precision. However, doing more changes than necessary could lead to loss of valuable simulation information gathered so far. If the mesh is really strongly distorted, e.g. containing the "hourglass-shaped" ($\bowtie$) quadrilateral cells, one first needs to untangle it, that is to fix all the fully or partly inverted elements. An efficient method to do this is the three-step algorithm [3], combining direct node placement based on geometrical considerations with numerical optimization of a quadratic functional which serves as a local mesh quality indicator. Another option is to prevent evolution of strong deformations (tangling) by regular use of a less expensive rezoning technique, such as the simple Winslow approach [2], where new node positions are given by

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

with coefficients $\alpha^k = x_\xi^2 + y_\xi^2$, $\beta^k = x_\xi\ x_\eta + y_\xi\ y_\eta$, $\gamma^k = x_\eta^2 + y_\eta^2$, where z_ξ, z_η denote finite differences in logical, index coordinates $z_\xi = (z_{i+1,j} - z_{i-1,j})/2, z_\eta = (z_{i,j+1} - z_{i,j-1})/2$. A more sophisticated method is based on the local parametrization and optimization of the Reference Jacobian matrix [4, 5]. First, each node is assigned a virtual reference position $\vec{x}^{(R)}$ by optimization of a local mesh quality estimator in its neighborhood. In particular, in N dimensions, for node V one minimizes the functional

$$Q_V = \sum_{T \in T_V} \|\mathbf{J}_{V,T}\| \cdot \|\mathbf{J^{-1}}_{V,T}\|,$$

which is a sum of condition numbers of the Jacobi mapping matrices

$$\mathbf{J}_{V,T} = [e_{V,1}, e_{V,2}, \ldots, e_{V,N}]$$

given by edges $e_{V,k} = \vec{x}_k - \vec{x}_V$ forming a virtual simplex in the N-dimensional space. The sum is taken over all simplices T sharing node V as a vertex. Then, global optimization is used to find a mesh of good quality, with edges as close as possible to their reference counterparts. This is done by minimization of the functional

$$F_{RJ} = \sum_V \sum_{T \in T_V} \frac{\|\mathbf{J}_{V,T}(x) - \mathbf{J^{(R)}}_{V,T}\|}{\|\mathbf{J^{(R)}}_{V,T}\|},$$

where the sum is taken over all mesh vertices V and the reference Jacobian matrix is defined as

$$\mathbf{J^{(R)}}_{V,T} = \left[e_{V,1}^{(R)}, e_{V,2}^{(R)}, \ldots, e_{V,N}^{(R)} \right], \qquad e_{V,k}^{(R)} = \vec{x}_k - \vec{x}_V^{(R)}.$$

Both functionals are optimized using the conjugate gradient method, which is well suited for problems with large number of parameters.

The input mesh for this procedure must not contain inverted elements (i.e. simplices with negative volume in the sense of original orientation). Therefore, strongly distorted meshes must be preprocessed by an untangling procedure, e.g. the three-step method [3] mentioned above.

4. Conservative transfer of solution (remapping)

Once the mesh is adapted (rezoned), the discrete values of conserved variables must be transferred (remapped) from the old mesh to this new, rezoned one. This procedure is required to be conservative for mass, each component of momentum,

and total energy and must preserve monotonicity (or at least local bounds) for density, velocity and specific internal energy. The remapping should be as accurate as possible. Exact transfer from the old mesh to the new one is required for linear functions. All this is achieved by a method which first interpolates discrete values by a piecewise linear function, then integrates it over swept regions and finally corrects the possibly created overshoots or undershoots by redistribution of these into the neighboring cells (so-called Repair) [11, 12].

Other techniques enforce all imposed requirements already during the remapping process, with no need of a posteriori repair. Many of them combine low-order intercell fluxes (which preserve local bounds by default) with some portion of higher-order (generally unconstrained) fluxes. An example called Flux-Corrected Remapping (FCR) is described in [13].

5. Numerical example

As a practical example, we show a simulation inspired by an experiment performed recently at the Prague Asterix Laser System (PALS) facility: a laser-irradiated aluminum disc ablatively accelerates and strikes a massive aluminum target [14, 15]. Here we focus on the second part, that is on disc impact. The setup is as in Fig. 1(a)

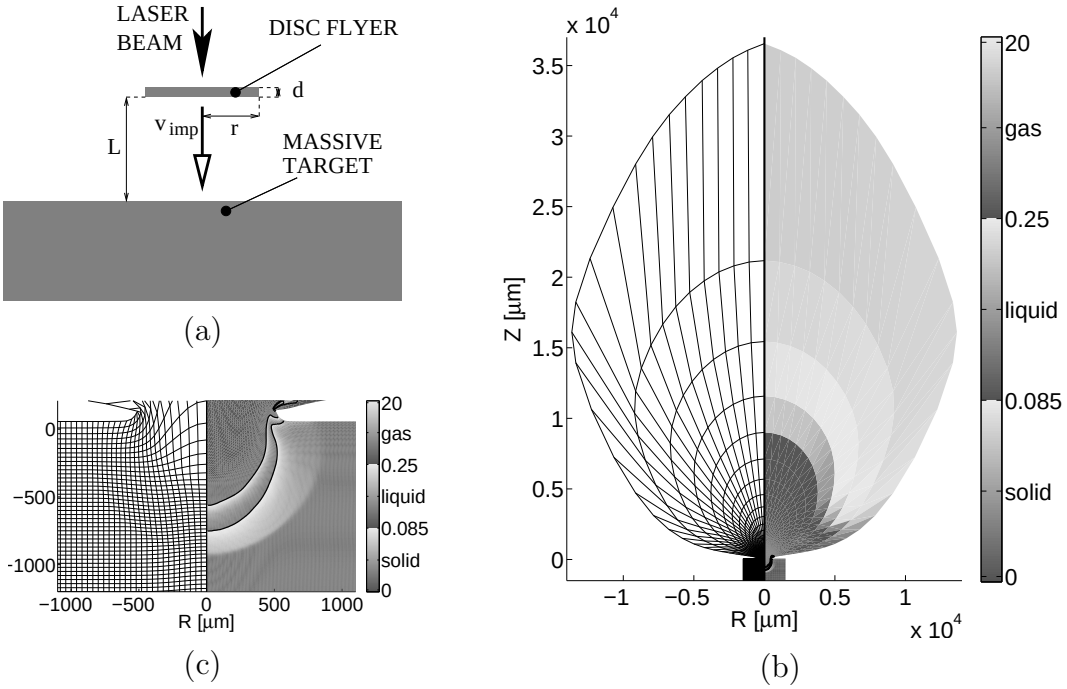

Fig. 1: *Disc impact problem. Experiment setup (a) and temperature at* 80 ns*: whole domain with hot plasma corona (b), detail of crater evolving in the target (c). Only every fourth layer of edges is shown in (c). Solid, liquid and gas phases are shown in separate colormaps.*

with the following parameters: a 400 ps laser pulse with energy 240 J operating in the 3rd harmonic with radius of focal spot on target $r_f = 125\,\mu$m, irradiates a $d = 11\,\mu$m thick disc with radius $r = 150\,\mu$m, located $L = 200\,\mu$m above the target. The disc is ablatively accelerated up to the impact velocity $v_{\mathrm{imp}} = 134\,$km/s and hits the target. Simulation starts at the moment of impact. Pure Lagrangian computation fails very soon (at approximately $t \approx 0.5\,$ns) because of fatal mesh distortion, while the ALE simulation preserves sufficient mesh quality for the computation to continue. In particular, EOS for ideal gas was used, mesh rezoning was performed by Winslow smoothing (2) and remapping by linear interpolation with Repair. The flyer starts to sink into the target, material of both the flyer and the target are compressed, heated and evaporated. Part of the hot material is ionized, ablated and forms an expanding plasma corona, shown at $t = 80\,$ns in Fig. 1(b). Shock wave is propagating into the target, continuing to melt and evaporate its material, see Fig. 1(c), where only every fourth mesh edge in each direction is shown, so that each quadrilateral corresponds to sixteen real cells. Solid, liquid and gas phases are shown by different colormaps in grayscale. In all performed tests, size and shape of the crater approximated the experimental data with reasonable precision.

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