

On using discontinuous finite element methods to simulate inertial confinement fusion

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SUMMARY

This paper is devoted to the simulation of inertial confinement fusion for target design. An arbitrary Lagrangian Eulerian formulation based on discontinuous Galerkin finite element methods is proposed. It is totally different from Wilkins' scheme used in traditional ICF codes. The objective here is to test the robustness of the method on non-uniform moving grids. The emphasis is put on the preservation of the spherical symmetry. Copyright © 2005 John Wiley & Sons, Ltd.

KEY WORDS: hydrodynamics; ALE; discontinuous finite elements

1. INTRODUCTION

This work is devoted to the development of codes to simulate inertial confinement fusion (ICF) experiments. Among the main difficulties in such simulations is the large variety of equations to be solved (the equations of compressible hydrodynamics, heat conduction, radiation transport, laser energy deposition) and the high compression ratios to be treated ($\Delta\rho/\rho \simeq 1000$). Moreover, multiple real materials with complex equations of state are present. In developing numerical schemes, we look for the robust methods and their ability to preserve the spherical symmetry of flows.

ICF implosion codes have traditionally used a two-dimensional, cylindrically symmetric, finite volume, Lagrangian hydrodynamics algorithm developed in the 1960s at LLNL [1]. Vertices move with the fluid to keep the element mass constant in time. The density and pressure are assumed to be uniform within each element, while the velocity is assumed to be a bilinear function of the vertex values. An artificial viscous force is included to broaden

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shocks, and a numerical processing—typically a velocity correction—is added to damp Hourglass motions.

This kind of approach presents several defects. First, it is really difficult to derive convenient viscosity terms: most of the artificial viscous forces are not derived from a proper tensor stress, and the resulting methods exhibit bad performances on meshes with large aspect ratio. Next, there is intrinsically a problem in using a staggered grid concerning the total energy, which is the sum of the internal energy located in the cell centres and the kinetic energy centred at the nodes. Finally, when most hydrodynamic calculations give rise to premature breakdown of the grid topology, the Lagrangian phase is followed by a rezoning step. A remapping phase is then required to interpolate the solution onto the improved mesh. There are difficult issues concerning the derivation of remapping algorithms that are second-order accurate, conservative and sign preserving.

This work is an attempt to propose another numerical scheme for hydrodynamics. An arbitrary Lagrangian Eulerian (ALE) formulation will be considered to relax the mesh in the presence of excessive grid distortions. The spatial discretization is based on the discontinuous Galerkin (DG) method. Its good performances are now well established for an Eulerian description of fluid motion [2, 3] and recent research on moving grids is very encouraging [4].

The first part of the paper presents the ALE formulation of hydrodynamics. The second part deals with spatial discretization. The emphasis is put on the verification of the geometric conservation law (GCL), which has been proven to be very important for time accuracy and stability properties [5]. The last part is devoted to numerical simulations.

2. THE ALE HYDRODYNAMICS EQUATIONS

2.1. Notations

Let $\Omega_0 \subset \mathbb{R}^2$ be a reference configuration (typically the domain position at the beginning of the simulation), and $\Omega_t \in \mathbb{R}^2$ an instantaneous configuration, with $t \in [0, T]$. A point in Ω_0 (respectively Ω_t) is denoted by $x^0 = (x_i^0)_{i=1,2}$ (respectively, $x = (x_i)_{i=1,2}$). At each time $t \in [0, T]$, a point $x^0 \in \Omega_0$ is associated to a point $x = x(x^0, t) \in \Omega_t$. Let $J_t = \partial x / \partial x^0$ be the Jacobian of the map. Traditionally, x^0 is called the ALE co-ordinate and x the spatial or Eulerian co-ordinate. The time derivative in the ALE frame written in the spatial co-ordinate is $Df/Dt = \partial f / \partial t + \omega_g \cdot \nabla_x f$, where $\omega_g(x, t) = Dx/Dt$ is the displacement velocity of the domain.

2.2. Governing equations

The ALE formulation of two-dimensional compressible fluid can be written as

$$\frac{D}{Dt} (J_t W) + J_t \nabla_x \cdot (F(W) - \omega_g W) = 0 \quad (1)$$

with initial and boundary conditions. The vector of conservative variables $W \in \mathbb{R}^4$, and the flux function $F = (F_1(W), F_2(W)), F_i(W) \in \mathbb{R}^4$ are defined as follows:

$$W = \begin{pmatrix} \rho \\ \rho u_1 \\ \rho u_2 \\ \rho E \end{pmatrix}, \quad F_1 = \begin{pmatrix} \rho u_1 \\ \rho u_1^2 + P \\ \rho u_1 u_2 \\ u_1(\rho E + P) \end{pmatrix}, \quad F_2 = \begin{pmatrix} \rho u_2 \\ \rho u_1 u_2 \\ \rho u_2^2 + P \\ u_2(\rho E + P) \end{pmatrix} \quad (2)$$

In (2), ρ is the mass density, ρu_i the momentum density, ρE the total energy density and P the pressure. The total energy per unit mass E is linked to the internal energy per unit mass I by the relation $E = I + \frac{1}{2} u_i u_i$. To close the system, an equation of state gives $I = I(\rho, P)$.

3. A DISCONTINUOUS FINITE ELEMENT APPROACH

3.1. Preliminaries

The 2D problem domain is meshed into an arbitrary and unstructured set of non-overlapping cells (triangular and/or quadrilateral elements). Within each element E , the solution $W_h(x, t)|_E$ is approximated by a polynomial of degree 1. There is no requirement of continuity across edges between elements. The mesh velocity is a linear or bilinear function of the vertex values (according to the element shape).

3.2. The semi-discretization in space

Equation (1) are multiplied by a test function φ_h and integrated on each element $E(0)$ of the initial configuration. Integrals are then transformed into the arbitrarily moving reference frame. The volume integral is integrated by parts twice to get

$$\begin{aligned} \frac{d}{dt} \int_{E(t)} \varphi_h W_h \, dv + \int_{E(t)} \varphi_h \nabla_x \cdot (F(W_h) - \omega_g W_h) \, dv \\ + \int_{\partial E(t)} \Phi(W_{hE}, W_{hE'}, \omega_g, n) \varphi_h \, d\sigma - \int_{\partial E(t)} (F(W_h) - \omega_g W_h) \cdot n \varphi_h \, d\sigma = 0 \end{aligned} \quad (3)$$

Upwinding is achieved by a numerical flux $\Phi(U, V, \omega_g, n)$ which results from the resolution of a local Riemann problem in the direction that is normal to the interfaces. It is conservative and consistent with the flux: $\Phi(U, U, \omega_g, n) = (F(U) - \omega_g U) \cdot n$. In (3), E' is the element sharing an edge with E . This is not the most commonly used approach but it makes the obtention of the GCL trivial. Finally, it is important to notice that a limiting procedure is necessary to impose a local maximum principle.

3.3. The geometric conservation law

The GCL states that the computation of the geometric parameters must be performed in such a way that, independent of the mesh motion, the resulting numerical scheme preserves the

state of a uniform flow. A misrepresentation of the convective fluxes due to an inaccurate calculation of geometrical quantities can result in numerical instabilities and oscillations [6]. Furthermore, real significance of those conditions in terms of scheme stability properties and time accuracy have been proposed by several authors [5].

We substitute a constant function W into the discrete system (3) and we look for conditions to be satisfied such that a constant field is an exact solution of the numerical scheme independent of the mesh velocity. We get after trivial manipulations

$$\frac{d}{dt} \int_{E(t)} \varphi_k \, dv = \int_{E(t)} \varphi_k (\nabla_x \cdot \omega_g) \, dv \quad (4)$$

It is supposed that the spatial volume integrals are computed exactly by using appropriate quadrature formulae. Consequently, the GCL is satisfied if the time integration of the term involving the mesh velocity divergence is exact.

Following Reference [7], we consider $E(t^n)$ as the reference configuration

$$A_{t^n} : \begin{matrix} E(t) & \longrightarrow & E(t^n) \\ x & \longmapsto & y \end{matrix} \quad (5)$$

We have $\hat{\varphi}(y) = \varphi \circ A_{t^n}(x)$, and we denote by J_{cof} the co-factor matrix of the ALE mapping. We get

$$\int_{E(t)} \varphi_k (\nabla_x \cdot \omega_g) \, dv = \int_{E(t^n)} \hat{\varphi}_k(y) (J_{\text{cof}} \nabla_y) \cdot \hat{\omega}_g \, dv$$

If the domain displacement is taken to be a piecewise constant polynomial in time, the co-factor matrix would be a polynomial in time $[t^n, t^{n+1}]$ of degree 1. Consequently, the GCL condition is satisfied once a one-point integration scheme of exactness one is used.

4. NUMERICAL EXPERIMENTS

Unities are expressed in the CGS system. All the numerical results have been obtained with a second-order scheme. The limiting procedure is based on the minmod function. It is an extension of the method of Cockburn and Shu [2] developed for triangles to the case of unstructured meshes of quadrilateral elements. Our objective was to test the DG scheme on an almost Lagrangian formulation. The mesh velocity has been computed from the fluid velocity by a simple average procedure. This point needs further analysis to limit as much as possible the mass flux at element interfaces, but it was adequate for the present study.

4.1. A modified Saltzman problem

The problem consists in solving a one-dimensional problem on a non-uniform two-dimensional mesh [8]. The initial mesh is composed by 100×10 cells. To damage the mesh aspect ratio, the computational domain is taken as $\Omega = [0, 1] \times [0, 1]$ in place of $[0, 1] \times [0, 0.1]$ as most authors do. Initially the gas is at rest with density 1 and zero pressure. The piston at the left moves with speed 10^8 . Figure 1 shows the density profiles at time 6×10^{-9} s of the solutions computed with the proposed scheme and the Wilkins' scheme. The DG scheme almost preserves the unidimensional symmetry. The solution obtained with the scheme of Wilkins

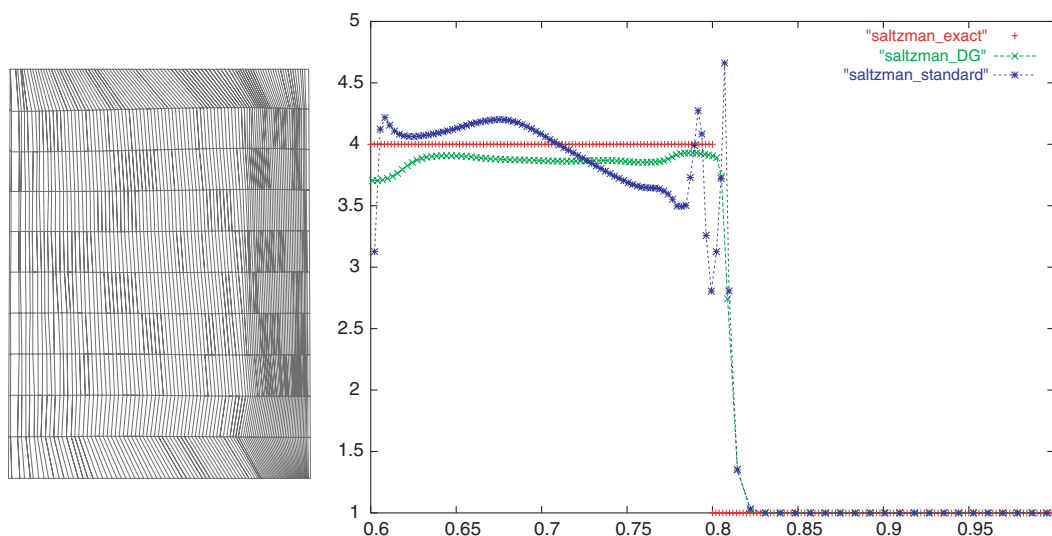


Figure 1. Saltzman problem. Mesh and density profiles at time 9.7×10^{-9} s. Exact solution, solution with the DG scheme and solution with the scheme of Wilkins.

could be improved by using a velocity correction to suppress Hourglass-type motions. But the objective here was to test the presence (or not) of non-physical modes in the DG approximate solution. Results are very good (see a portion of the mesh at time after one reflection on the right-hand wall).

4.2. Compression of a sphere

We study the deformation of a sphere, composed of two materials, submitted to a force on its outer boundary. We have considered a 10×10 polar grid with initially equal radial and angular interval. Initially, the radius of the outer boundary is 1. The pressure is 1.2515518×10^{-2} . The density of the internal material ($0 \leq r \leq 0.5$) is 1 and the density of the external material ($0.5 \leq r \leq 1$) is 4. The compression is driven by imposing a pressure of 10 on the external boundary. The solution at time 0.3 is represented in Figure 2. The symmetry of the problem is well preserved.

4.3. The Noh problem

In this problem, we study a shock reflecting from an axis in a convergent geometry [9]. It is computed in a quarter plane with reflective boundary conditions on both axes. The initial grid is uniform and is 50×50 . Initially, the density is 1, the pressure is 0 and the velocity is directed towards the centre with magnitude 1. We have represented a mesh portion at the final time and the density profiles along the two axes (see Figure 3). Solutions have density profiles with a large disparity from the analytical result because the mesh convergency is not reached, but the spherical symmetry of the problem is well preserved. The phenomenon of 'wall heating' [9] near the axis is common to any scheme based on Lagrangian formulation. The mesh after the shock reflection is particularly good.

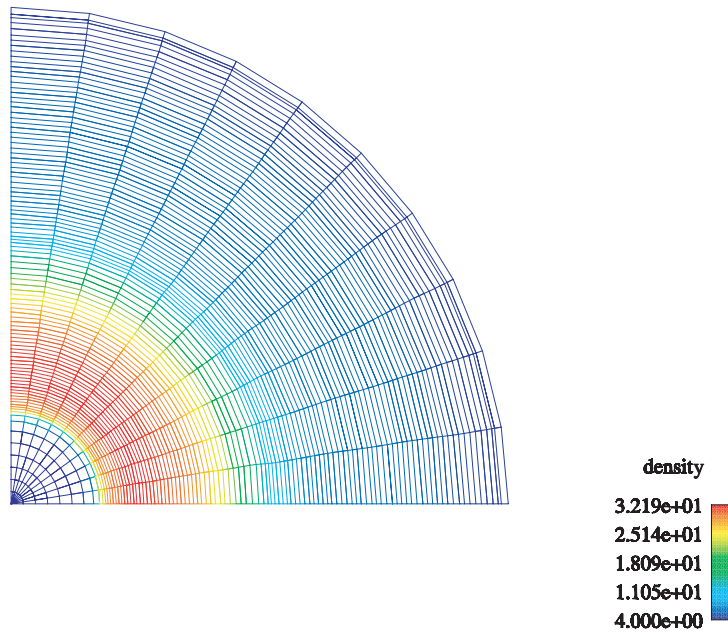


Figure 2. Compression of a sphere. Isolines for density at time 0.25 s.

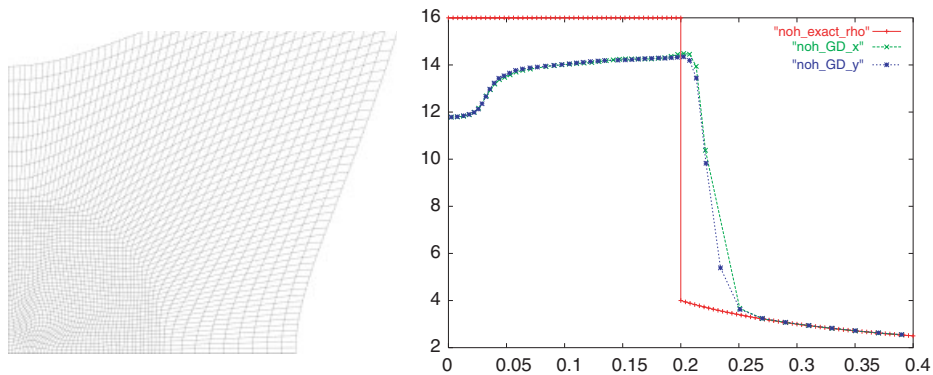


Figure 3. The Noh problem. Portion of the mesh and density profiles.

5. CONCLUSIONS

This preliminary study is very encouraging for the development of discontinuous finite element schemes for ICF codes. We have obtained the same conclusions as Kershaw *et al.*, i.e. this is a very interesting alternative to simulate flows with very high aspect ratios in converging geometries. The on-going work is devoted to the improvement of the limiting procedure which is not fully satisfactory on spherical configurations meshed by quadrilaterals.

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