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Positivity-preserving cell-centered Lagrangian schemes for multi-material compressible flows: From first-order to high-orders. Part I: The one-dimensional case

François Vilar [a,*], Chi-Wang Shu [a], Pierre-Henri Maire [b]

[a] Division of Applied Mathematics, Brown University, Providence, RI 02912, USA
[b] CEA/CESTA, 15 Avenue des Sablières CS 6001, 33 116 Le Barp cedex France

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ABSTRACT

One of the main issues in the field of numerical schemes is to ally robustness with accuracy. Considering gas dynamics, numerical approximations may generate negative density or pressure, which may lead to nonlinear instability and crash of the code. This phenomenon is even more critical using a Lagrangian formalism, the grid moving and being deformed during the calculation. Furthermore, most of the problems studied in this framework contain very intense rarefaction and shock waves. In this paper, the admissibility of numerical solutions obtained by high-order finite-volume-scheme-based methods, such as the discontinuous Galerkin (DG) method, the essentially non-oscillatory (ENO) and the weighted ENO (WENO) finite volume schemes, is addressed in the one-dimensional Lagrangian gas dynamics framework. After briefly recalling how to derive Lagrangian forms of the 1D gas dynamics system of equations, a discussion on positivity-preserving approximate Riemann solvers, ensuring first-order finite volume schemes to be positive, is then given. This study is conducted for both ideal gas and non-ideal gas equations of state (EOS), such as the Jones–Wilkins–Lee (JWL) EOS or the Mie–Grüneisen (MG) EOS, and relies on two different techniques: either a particular definition of the local approximation of the acoustic impedances arising from the approximate Riemann solver, or an additional time step constraint relative to the cell volume variation. Then, making use of the work presented in [89,90,22], this positivity study is extended to high-orders of accuracy, where new time step constraints are obtained, and proper limitation is required. Through this new procedure, scheme robustness is highly improved and hence new problems can be tackled. Numerical results are provided to demonstrate the effectiveness of these methods.

This paper is the first part of a series of two. The whole analysis presented here is extended to the two-dimensional case in [85], and proves to fit a wide range of numerical schemes in the literature, such as those presented in [19,64,15,82,84].

* Corresponding author.
E-mail addresses: francois.p.vilar@gmail.com (F. Vilar), shu@dam.brown.edu (C.-W. Shu), maire@celia.u-bordeaux1.fr (P.-H. Maire).

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1. Introduction

This paper is the first part of a series of two, which is only concerned with the one-dimensional case. The second paper, [85], investigates the two-dimensional situation. Here, we aim at demonstrating the positivity-preservation property of methods solving one-dimensional Lagrangian gas dynamics equations, from first-order to high-orders of accuracy, under suitable constraints.

It is well known that fluid dynamics relies on two kinematics descriptions: the Eulerian or spatial description and the Lagrangian or material description, refer for instance to [49,44]. In the former, the conservation laws are written using a fixed reference frame whereas in the latter they are written through the use of a time dependent reference frame that follows the fluid motion. The Lagrangian representation is particularly well adapted to describe the time evolution of fluid flows contained in regions undergoing large shape changes due to strong compressions or expansions. Further, in this approach, there is no mass flux across the boundary surface of a control volume moving with the fluid velocity. Thus, Lagrangian representation provides a natural framework to track accurately material interfaces in multi-material compressible flows. Moreover, such a representation avoids the appearance of numerical diffusion resulting from the discretization of the convection terms present in the Eulerian framework.

In the Lagrangian description, the gas dynamics system may be derived in two different but consistent formulations, namely the updated Lagrangian formulation based on the moving configuration, and the total Lagrangian formulation based on the fixed initial configuration. In this latter approach, the physical conservation laws are written employing the Lagrangian coordinates which refer to the initial configuration of the fluid flow. Moreover, in these equations the divergence and gradient operators are expressed by means of the Piola transformation [49], which requires the knowledge of the deformation gradient tensor, *i.e.* the Jacobian matrix associated to the Lagrange–Euler flow map. The deformation gradient tensor characterizes the time evolving deformation and is governed by a partial differential equation named the geometric conservation law (GCL). To ensure the consistency between the initial and the current configurations, this tensor has to satisfy an involutive constraint [73], which implies the Piola compatibility condition. The total Lagrangian approach is very well known in the solid mechanics community wherein it is extensively used to model solid dynamics undergoing large deformations [49]. In contrast to the total Lagrangian formulation, the updated Lagrangian formulation is a moving domain method, which is widely employed in fluid mechanics. In this approach, the gas dynamics equations are written employing the Eulerian coordinates. They refer to the current configuration of the fluid flow. The time derivative of the physical variables is taken following the path of the fluid particles: this is the material derivative. The integral formulation of the conservation laws is readily obtained by employing the Reynolds transport formula over an arbitrary moving control volume. The time rate of change of a zone volume is governed by a partial differential equation which is the updated Lagrangian form of the GCL.

Two approaches are mainly employed to solve updated Lagrangian formulations of the gas dynamics equations, namely the cell-centered and staggered approaches. In the cell-centered hydrodynamics, a cell-centered placement of all hydrodynamic variables is employed. However, the referential being assumed to move as the fluid flows, one needs to advect the grid points. Also, this has to be done with respect to the GCL, which means that the new volume computed through the new position of the grid nodes has to be the same as the one derived from the discretization of the governing equation of the specific volume. Furthermore, in the multi-dimensional case, due to the large number of neighboring cells sharing a node, one cannot apply in a straightforward manner one-dimensional solvers to define uniquely the grid point velocity. The staggered hydrodynamics has been developed to avoid such complications. In this framework, a staggered discretization is employed such that the kinematic variables (vertex position, velocity) are located at the nodes whereas the thermodynamic variables (density, pressure, internal energy) are defined at the cell centers. The conversion of kinetic energy into internal energy through shock waves, consistent with the second law of thermodynamics, is ensured by adding an artificial viscosity term. The staggered grid schemes employed in most hydro-codes have been remarkably successful over the past decades in solving complex multi-dimensional compressible fluid flows, refer for instance to [45,88,17,18,32,55,33,34,4]. However, they clearly have some theoretical and practical deficiencies such as mesh imprinting and symmetry breaking. In addition, the fact that all variables are not conserved over the same space can make these schemes difficult to handle when one wants to assess analytical properties of the numerical solution. For all these reasons, this paper focuses on the cell-centered approach. Different techniques may be employed to build the numerical fluxes and move the grid through the use of approximate Riemann solvers, with respect to the GCL. The interested readers may refer to the following papers [1,19,20,61, 72,15,53,82,5,16,10,84] for a more detailed description of this approach and its variants. Let us mention that besides these two mainly employed approaches, *i.e.* the cell-centered and staggered approaches, a third one has recently grows quickly in popularity these past years. This third framework, referred to as Point-Centered Hydrodynamic (PCH), combines the features of the first two, namely a dual grid and the fact that kinetical and thermodynamical variables are conserved on the same cells. Indeed, in this particular frame, the momentum and total energy conservation equations are solved on the dual grid around the nodes, generally by means of an edge-based finite element scheme or an edge-based upwind finite volume method. The PCH approach has been successful applied these past decades to problematics concerned with the simulation of incompressible flows, compressible Lagrangian flows, or Lagrangian solid dynamics, refer for instance to [28,29,24,42,48, 76,79,78,86,87,67,68,2,3]. Two of the main advantages of these schemes are that there are very well adapted to triangular or tetrahedral grids, as well as they reduce in most cases problems related to mesh stiffness.