Available online at www.sciencedirect.com
ScienceDirect
Journal of Computational Physics 218 (2006) 572–593
JOURNAL OF COMPUTATIONAL PHYSICS
www.elsevier.com/locate/jcp

The internal consistency, stability, and accuracy of the discrete, compatible formulation of Lagrangian hydrodynamics

A.L. Bauer [a,b,*], D.E. Burton [c], E.J. Caramana [d], R. Loubère [e], M.J. Shashkov [b], P.P. Whalen [f]

[a] *Department of Mathematics, University of Michigan, 2074 East Hall, 530 Church Street, Ann Arbor, MI 48109-1043, USA*
[b] *T-7, MS B284, Los Alamos National Laboratory, Los Alamos, NM, USA*
[c] *X-3, MS T086, Los Alamos National Laboratory, Los Alamos, NM, USA*
[d] *CCS-2, MS D413, Los Alamos National Laboratory, Los Alamos, NM, USA*
[e] *MIP, University of Toulouse, 31062 Toulouse Cedex 9, France*
[f] *X-7, MS F644, Los Alamos National Laboratory, Los Alamos, NM, USA*

Received 30 November 2005; received in revised form 21 February 2006; accepted 23 February 2006
Available online 19 April 2006

Abstract

This work explores the somewhat subtle meaning and consequences of the salient properties of the discrete, compatible formulation of Lagrangian hydrodynamics. In particular, since this formulation preserves total energy to roundoff error, the amount of error in the conservation of total energy cannot be used to gauge the internal consistency of calculations, as is often done with the older forms of this algorithm. However, the compatible formulation utilizes two definitions of zone volume: the first is the usual definition whereby the volume of a zone is defined as some prescribed function of the coordinates of the points that define it; the second is given as the integration in time of the continuity equation for zone volume as expressed in Lagrangian form. It is the use of this latter volume in the specific internal energy equation that enables total energy to be exactly conserved. These two volume definitions are generally not precisely equal. It is the analysis of this difference that forms the first part of this study. It is shown that this difference in zone volumes can be used to construct a practical internal consistency measure that not only takes the place of the lack of total energy conservation of the older forms of Lagrangian hydrodynamics, but is more general in that it can be defined on a single zone basis. It can also be used to ascertain the underlying spatial and temporal order of accuracy of any given set of calculations. The difference in these two definitions of zone volume may be interpreted as a type of entropy error. However, this entropy error is found to be significant only when a given calculation becomes numerically unstable, otherwise it remains at or far beneath truncation error levels. In fact, it can be utilized to provide an upper bound on the size of the spatial truncation error for a stable computation. It is also shown how this volume difference can be used as an indicator of numerical difficulties, since exact local conservation of total energy does not guarantee numerical stability or the quality of any numerical calculation. The discrete, compatible formulation of Lagrangian hydrodynamics utilizes a two level predictor/corrector-type of time integration scheme; a stability analysis, both analytical and numerical, is given. This analysis reveals a novel stability diagram

* Corresponding author. Tel.: +1 734 936 4557/997 0509; fax: +1 734 763 0937.
E-mail addresses: albauer@umich.edu (A.L. Bauer), burton@lanl.gov (D.E. Burton), ed.caramana@gmail.com (E.J. Caramana), loubere@mip.ups-tlse.fr (R. Loubère), shashkov@lanl.gov (M.J. Shashkov), ppw@lanl.gov (P.P. Whalen).

0021-9991/$ - see front matter
doi:10.1016/j.jcp.2006.02.024

that has not been heretofore published, and gives definitive information as to how the stabilizing corrector step should be centered in time.

Keywords: Lagrangian scheme; Stability; Compressible fluids; Compatible discretization; Support operator

1. Introduction

The Lagrangian formulation of the equations of hydrodynamics has a very old and venerable history. Indeed, the very first large-scale numerical calculations that resemble modern computer simulations in both complexity and in the numerical issues considered utilized fluid equations in the Lagrangian frame of reference in one-dimension [1]. If one considers an arbitrary fluid velocity v and distinct sound speed c_s, then in one-dimension the characteristic trajectories of the fluid equations have associated eigenvalues $v \pm c_s$ and v. In the Lagrangian frame that follows the fluid velocity v, these eigenvalues transform into the Galilean invariant values $\Delta v \pm c_s$ and Δv, where Δv is the difference in velocity between two adjacent discrete spatial locations in the flow field. Thus, the Lagrangian frame of reference is unique, and one characteristic is chosen and followed exactly, except for spatial gradients in the velocity field. The fact that the Lagrangian description of fluid dynamics is automatically adaptive makes it the preferred representation in one-dimension. Newton's second law of motion, $\vec{F} = M\vec{a}$, where M is the mass of a point particle (or fluid element), $\vec{F}$ is the total force acting on it, with the acceleration $\vec{a}$ given as the second derivative with respect to time of its displacement vector $\vec{r}$, is a statement set in the Lagrangian frame of reference. Discretizing this equation directly with respect to time utilizing $\vec{r}$ as a dependent variable results quite naturally in the three-level leapfrog scheme. These time levels are usually denoted as $n-1$, n, and $n+1$, with the force $\vec{F}$ spatially differenced in some manner but placed at time level n. All early Lagrangian algorithms in both 1D [2] and in 2D [3] utilized this kind of discretization with respect to time. Although this forms a simple and intuitive numerical integration scheme, it leaves the velocity of a mass point or fluid element defined only as the difference between its displacement vector at two different time levels, and therefore the velocity is defined only at the $n \pm \frac{1}{2}$ time levels. When one then considers the total energy of a fluid as a sum of both kinetic energy and internal energy that can be exchanged between each other by the action of forces, this sum is difficult to conserve exactly in discrete form owing to the fact that the two components that comprise it are defined at different time levels. When velocity dependent forces are explicitly added to this model, as with the artificial viscosity [4], this type of time integration becomes somewhat clumsy and looks even contrived [2], since the artificial viscosity terms must be lagged in time to preserve numerical stability.

The spatial discretization of the force in all early versions of Lagrangian hydrodynamics [2,3] is some form of what is presently known as finite-volume differencing. That is, these various forms calculate force as a stress (scalar pressure plus deviators) times a normal surface-area vector. The most modern of these older force calculations is the diamond differencing scheme due to Wilkins [3], which uses closed surface area contours to calculate the force acting on a point, and thus properly conserves linear momentum in a trivial manner. Others piece the force contributions together in various ways to form the total force acting on each fluid element such that strict conservation of linear momentum may, or may not, be obtained. Most Lagrangian hydrodynamics codes employ a spatially staggered placement of dependent variables with stress, density, and specific internal energy given in zones surrounded by points that have associated position and velocity vectors. This enables the calculation of forces by means of the various kinds of finite-volume differencing referenced above, with masses and volumes ascribed to both zones and points in an interleaved manner. This also avoids the "grid-decoupling" instability that is the bane of non-staggered forms of this algorithm. A difficulty with the older work is that there was no agreement amongst the various authors of these different algorithms as to how these schemes, aside from the noted common features, should be constructed. The choices made were largely arbitrary and not tied to solid mathematical concepts.

An early attempt to remedy this lack of a sound theoretical basis is the work of Goad [5], who used the method of virtual work to derive a form of finite-volume force differencing of the stress in 2D cylindrical