Issues of an Eulerian/ALE Algorithm Based on a Compatible, Staggered-Grid, Lagrangian Step

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1 Introduction

In this paper a number of distinct issues that are of concern in the construction of an Eulerian or ALE algorithm by means of a Lagrangian step and separate remap are explored. First, the common advection test problems usually cited in the literature pertaining to limiter construction are not wholly suitable to accessing the advection quality of an Eulerian scheme. A more appropriate set of test problems are derived to satisfy this need. Next, the basic philosophy of an ALE algorithm is that it should function as close to the Lagrangian limit as possible, and should therefore approach that limit in a uniform manner. Certain difficulties with achieving this using a spatially staggered Lagrangian step (coordinates and velocity are point centered, density, internal energy, stresses, etc. are zone centered), particularly with regard to the update of subzonal pressure forces utilized in the Lagrangian step to control hourglass and other spurious grid motions, are discussed. An additional problem with the Lagrangian step occurs in 2D cylindrical geometry where so-called "area-weight" differencing is used to obtain the limit of 1D spherical symmetry. Here the nodal mass, and thus the momentum and kinetic energy, is formed by a particular construct that does not have any true volume associated with it. The proper treatment of this pecularity is given. Finally, advection on an unstructured grid may in certain instances be facilitated by means of an underlying structured one; situations where this may be preferred are briefly detailed.

2 Advection Test Problems

Advection test problems in the literature [1] are usually based on the equation for the advection of a passive scalar given as

$$\frac{d\rho}{dt} = \frac{\partial \rho}{\partial t} + \vec{V} \cdot \nabla \rho = 0 \,. \tag{1}$$

Here ρ is any scalar and is specified at time $t = 0$, whereas the velocity $\vec{V}(\vec{x}, t)$ is prescribed for all time and is incompressible, $\nabla \cdot \vec{V} = 0$. For an ALE algorithm that consists of a Lagrangian step plus a remap, it is useful to consider the limit of one-dimensional (1D) solutions where both compressibility and conservation of the amount of the advected scalar ρ are important.

Consider the continuity equation for the density ρ in the 1D limit as

$$\frac{\partial \rho}{\partial t} + \frac{1}{R^{\beta-1}} \frac{\partial}{\partial R} R^{\beta-1} V_R \rho = 0 \,, \tag{2}$$

where "R" is the radial coordinate and $\beta = 1, 2, 3$ gives cartesian, cylindrical, and spherical geometry, respectively. Let the boundary $R_b(t)$ move with time in some prescribed manner so that Eq.(2) is defined on the time varying domain $[0 \leq R < R_b(t)]$. Next, define $x = R/R_b(t)$, whence

$$\left.\frac{\partial}{\partial t}\right|_R = \left.\frac{\partial}{\partial t}\right|_x + \frac{dx}{dt}\frac{\partial}{\partial x} = \left.\frac{\partial}{\partial t}\right|_x - \frac{x}{R_b}\frac{dR_b}{dt}\frac{\partial}{\partial x} \,, \tag{3}$$

and Eq.(2) becomes

$$\left.\frac{\partial \rho}{\partial t}\right|_x - \frac{x}{R_b}\frac{dR_b}{dt}\frac{\partial \rho}{\partial x} + \frac{1}{R_b x^{\beta-1}}\frac{\partial}{\partial x} x^{\beta-1} V_R \rho = 0 \,, \tag{4}$$

defined on the fixed domain $[0 \leq x < 1]$. We now choose a simple, and thus integrable, form for the velocity $V_R(x,t)$ as

$$V_R(x,t) = -c x^{n+1} \,, \tag{5}$$

where the integer $n \geq 0$ to guarantee regularity as $x \to 0$. We choose the general boundary velocity function $c(t)$ to be a fixed positive constant that is set to unity, $c = 1$. Thus the motion of the outer boundary is

$$R_b(t) = 1 - t \equiv \tau \,, \tag{6}$$

where we also have set $R_b(t=0) = 1$. Using this equation to define the new time variable "τ", Eq.(4) has the simple linear form

$$\frac{\partial \rho}{\partial \tau} + \frac{(x^{n+1} - x)}{\tau}\frac{\partial \rho}{\partial x} + \frac{(n+\beta)x^n}{\tau}\rho = 0 \,, \tag{7}$$

which can be solved by the method of characteristics. This yields

$$\frac{d\tau}{\tau} = \frac{dx}{x(x^n - 1)} = -\frac{d\rho}{(n+\beta)x^n \rho} \,, \tag{8}$$

and using $\int \frac{dx}{x(1-x^n)} = \frac{1}{n} \ln \frac{x^n}{1-x^n}$ one has closed form solutions for $\rho(R,t)$ given the velocity profile of Eqs.(5,6). If one integrates along characteristics

to obtain some final coordinate R_f that began at location R_i at the initial time, then this result is found to yield a simple relation between the initial and final densities as

$$\rho(R_f) = \rho(R_i) \left(\frac{R_i}{R_f} \right)^{n+\beta} , \tag{9}$$

which can also be seen directly from Eq.(7) for the case where $n = 0$, as it becomes an ODE.

The case $n = 0$ is of particular interest because it corresponds to "self-similar" adiabatic motion. Consider the momentum equation in 1D Lagrangian form, written as

$$\rho \frac{d\vec{V}}{dt} = \rho \left(\frac{\partial V_R}{\partial t} + V_R \frac{\partial}{\partial R} V_R \right) = F_R \equiv 0 , \tag{10}$$

where the radial force $F_R = 0$. Then, Eq.(5) with $n = 0$ gives the radial velocity as

$$V_R(R,t) = \frac{-R}{1-t} , \tag{11}$$

which is also seen to satisfy the radial momentum equation, Eq.(10), with zero force. ($n = 0$ is the only case that does this.) Since by definition $V_R \equiv dR/dt$, Eq.(11) integrates to yield

$$R_f = R_i(1 - t_f) , \tag{12}$$

where $R_i = R(t = 0)$, $R_f = R(t = t_f)$, and $t_f < 1$. Thus, Eqs.(9,11,12) with $n = 0$ give the solution of the fluid equations with zero force for cartesian, cylindrical, and spherical geometry. The velocity is the same in all three cases but the density varies depending on geometry; also, note that both the density and velocity vary in magnitude with time. This leads us to propose the following set of test problems where not only ρ, but also V_R, is given only at the "initial" time. Thus one can guage not only the quality of ρ at a later time after advection through some number of zones, but also the quality of V_R, as well as conservation of mass, momentum, and kinetic energy (specific internal energy should remain zero). This form of advection test problem is more appropriate for accessing the quality of advection of an ALE scheme performed as a Lagrangian step plus remap, since the velocity is given at the beginning of the advection step, or here, at the initial time. Thus the problems of conservation of momentum and kinetic energy are present.

For definiteness we propose the following test problem:

Test Problem 1:

A sphere in 2D cylindrical (r, z) geometry.

Grid: one quadrant with domain $(0 \leq R \leq 1.1)$

Angular: $(0° \leq \theta \leq 90°)$ with $\Delta\theta \approx 30°$ (arbitrary really) $\Delta R = 1./400.$ (40 zones per 0.1 interval)

Square: $\Delta r = \Delta z = 1./400.$ and $0 \leq (r, z) \leq 1.1$

Initial Conditions:

$\rho = 1., V_r = -r, V_z = -z$ for $.95 \leq R \leq 1.05$ (40 zones) and $\rho = V_r = V_z = 0.$ elsewhere.

Note: $\vec{V}$ is undefined in regions where $\rho = 0.$ as can be seen from Eq.(10) (what we advect is momentum anyhow). The solution to Eq.(10) is "patched" together at $R = .95, R = 1.05$ and we choose to set $\vec{V} = 0.$ wherever ρ is at roundoff-error levels.

Solution: At times $t_f = 0.5, 0.75, 0.9$ the density from Eq.(9) with $\beta = 3, n = 0$ is $\rho = 8.0, 64.0, 1000.0$ centered about $R = 0.5, .025, 0.1$, and with a total spread of 20, 10, 4, zones radially, respectively, and zero or at roundoff level elsewhere. The non-zero velocity is given by Eq.(11) at the prescribed final times.

The above test problem can be easily modified to other geometries, resolutions and grid constructions in 2D or 3D; the initial density profile can be arbitrary but should have sufficient points to resolve it at the final time. A challange that this test problem presents is to obtain monotone behavior of both density and velocity at the leading and trailing edges of the initially square pulse. On a staggered spatial grid one advects momentum and mass, and with separate limiter functions, on different control volumes. The division of momentum by mass to obtain velocity does not guarantee monotonicity; also, it is necessary to set a cutoff at roundoff accuracy on density, where $\vec{V}$ is set to zero, to prevent this operation from becoming indeterminate. The advection step just described yields an implied kinetic energy that will not be equal to that found by advecting the kinetic energy directly as a separate scalar. Minimizing the magnitude of this difference is important to the quality of any advection algorithm.

3 Corner-Centering and Subzonal Pressure Forces

In the recent "compatible" formulation of Lagrangian hydrodynamics on a staggered spatial grid [2] a prominent role is given to corner objects, both masses and forces, that are defined with a dual reference to both a point "p" and a zone "z", where these integer indicies range over all points and zones of the grid. In this formulation the corner volume contains all variables, momentum and internal energy for instance, that were previously thought to be defined in different "staggered" spatial locations. In particular, it follows from the dual Lagrangian assumption used in both the momentum and internal energy equations, which are defined as piecewise constant over different but intersecting spatial locations as shown in Figure(1), that the corner mass m_p^z from which both the zone and point masses are constructed is itself "Lagrangian" [2]. This fact was the motivation for the construction of subzonal pressure forces that are due to the difference in density of the subzone volume ($\rho_z^p = m_z^p / v_z^p$) and that of the whole zone ($\rho_z = M_z / V_z$) [3].

The above mentioned emphasis on the importance of the subzone volume as the intersection of zone and point centered volumes gave rise to the idea that one should construct an Eulerian or ALE scheme by using the staggered Lagrangian step with a remap step that advects all quantities from the smaller (wrt a zone) corner volumes on which no spatial grid staggering appears. This was implemented and resulted in difficulties that are now discussed. First, one must obviously subcycle this advection step with respect to the Lagrangian timestep since the smaller subzone volume will advect potentially a larger fraction then that of the full zone, and the CFL timestep restriction on the Lagrangian step may be too large. Next, one must construct appropriate subzone limiter functions for mass, velocity, specific internal energy, etc. with respect to the subzone volumes, although one can initially use full upwinding as a first try. The problem one encounters with such a procedure is that the full density gradient now fills in across the subzones just as though these were separate zones themselves. Thus, while the density variation between subzones of a given zone is always found to be small for a pure Lagrangian algorithm (20% to 30% variation is very large), one finds that this change can become huge (factors of 2 to 4 about a strong shock). This undesirable property means that the pure Lagrangian limit cannot be taken uniformly as advection becomes small. Even a small amount of advec-

tion will produce large relative changes in the densities of the subzones of a given zone relative to that which one finds due to purely Lagrangian motion. Subzonal pressure forces now becomes large and no longer have the same interpretation that they did for a pure Lagrangian scheme. On Noh's problem, for instance, run in pure Lagrangian mode the subzonal density at the shock front shows a variation of about $3-4\%$ about the mean; behind the shock this relaxes to about $10^{-3}\%$. The result for the Eulerian scheme described shows a subzone density in zones behind the shock of about 50 and 70 with a mean of about 60. This large residual density variation within a zone is unacceptable. For this reason it was decided that subzonal advection is an untenable approach, and was given up on. The real problem appears to be that one must make a clear and well delineated distinction between "zones" and "subzones"; advection using subzone volumes smears this distinction too much and goes too far in making subzone volumes appear to be the same as what was the original zone volume, and with undesirable results.

If advection is performed on a zone basis there remains the question of how the subzonal density, differing from the mean zone density on the Lagrangian step, is to be modified. The subzonal pressure forces due to this difference are still needed, even in the Eulerian limit. The answer to this problem can be given in a very simple manner. Suppose that the Lagrangian step has just been completed so that updated volumes, and thus both zone and subzone densities, are known. In each zone define the factors f_z^p such that the subzone density ρ_z^p is related to its respective zone density ρ_z by

$$\rho_z^p \equiv (1 + f_z^p)\rho_z \; ; \tag{13}$$

the factors f_z^p are thus small numbers. Suppose that during the advection step an amount of mass δM_z enters zone "z" (mass that leaves a zone is not counted). We make the assumption that this entering mass is to be distributed uniformly throughout the zone. From this assumption the factors f_z^p associated with this zone are all relaxed toward zero as

$$f_z^{p,1} = f_z^p(1 - \delta M_z/M_z^1) \; , \tag{14}$$

where the superscript "1" denotes quantities after advection. Next, tentative subzone masses $m_z^{p,1}$ are defined as $m_z^{p,1} = \rho_z^1 V_z^{p,1}(1 + f_z^{p,1})$, where $V_z^{p,1}$ and ρ_z^1 are the after advection subzone volumes and mean zone density. Last the new subzone masses $m_z^{p,1}$ must be rescaled by a common factor so that when summed about all points "p" of the given zone "z" they yield the new

zone mass M_z^1. One can now proceed to the next Lagrangian step with new values for subzonal masses and densities. (These new subzone masses are also summed about a point to obtain the after-advection point mass M_p.) During the Lagrangian step the factors f_z^p may increase or decrease in magnitude depending on the evolution of the zone volume, while during the advection step they are only allowed to decrease in magnitude.

4 Advection with Area-Weight Differencing

Area-weight differencing is a particular kind of modified finite-volume algorithm that is used in 2D (r, z) cylindrical geometry to obtain the limit of 1D spherical symmetry on an equal-angle zoned (R, θ) grid. Various versions of this method have appeared over the last forty years that basically differ in their definition of the nodal mass, or areal-inertia, (see [4],[2] and references within). The basic idea is to make the momentum equation look like that in 2D cartesian geometry and introduce cylindrical effects only through the definitions of volume. A version of this algorithm was given in [2] where the nodal mass is Lagrangian, and thus can be made to exactly conserve total energy in the Lagrangian step (other versions do not obtain this). This was achieved by defining a nodal mass as a decomposition of the cylindrical zone mass into factors of density times area times the "r" coordinate r_p of the respective points "p" that define a given zone "z"; these corner masses are then summed to obtain a Lagrangian nodal mass that contains only density times area times a "common" r_p coordinate that then cancels everywhere in the momentum equation (forces are calculated analogously) to give a cartesian form that obeys the symmetry limit. In the remap step these nodal masses are useless for performing advection since they have no associated circumscribed volume.

The solution of how to perform advection in this case is simply to use the above mentioned nodal masses in the Lagrangian step but to define another set of "true" corner masses and associated nodal mass for use in the advection step (true corner masses are also used to define subzone densities in the Lagrangian step). These true corner masses and volumes are defined in the usual manner [2]. However, in switching mass definitions at the end of the Lagrangian step one changes the point momentum and kinetic energy because the point velocity is unchanged but the mass associated with it is modified (e.g., points on the z-axis of an area-weighted scheme carry zero mass). This

change in momentum and kinetic energy occurs again once the advection step is completed and one switches back to newly defined area-weight nodal masses to perform the next Lagrangian step. What is done in this case is to keep track of the changes in kinetic energy during these two steps and simply tally this so that a definition of proper total energy balance can be maintained. This is important because during the advection step kinetic energy can be lost since the seperate advection of mass, momentum, and kinetic energy are never directly consistent. A proper tracking of total energy and its constituent parts is necessary to the evaluation of any hydrodynamics algorithm.

5 Nondynamical Points in Advection

The remap step is more difficult to perform on unstructured grids where the zone topology can be arbitrary. Although unstructured grids may be necessary to zone complicated engineering structures, often they are used unnecessarily to overcome the problem of numerical and artificial spatial grid stiffness that will arise at a tappered end or a center of convergence of material regions. In this case an underlying logical grid composed of simple (and also degenerate) zones makes the associated remap step much easier to handle. We wish to point out that it is entirely unnecessary to use unstructured grids to overcome the spatial grid stiffness problem [5]; one can simply retain the underlying simple logical grid structure by introducing nondynamical points to eliminate spatial grid stiffness. The advection step in such situations is perfectly well behaved as far as timestep is concerned and can be performed with respect to the simple underlying structured grid.

References

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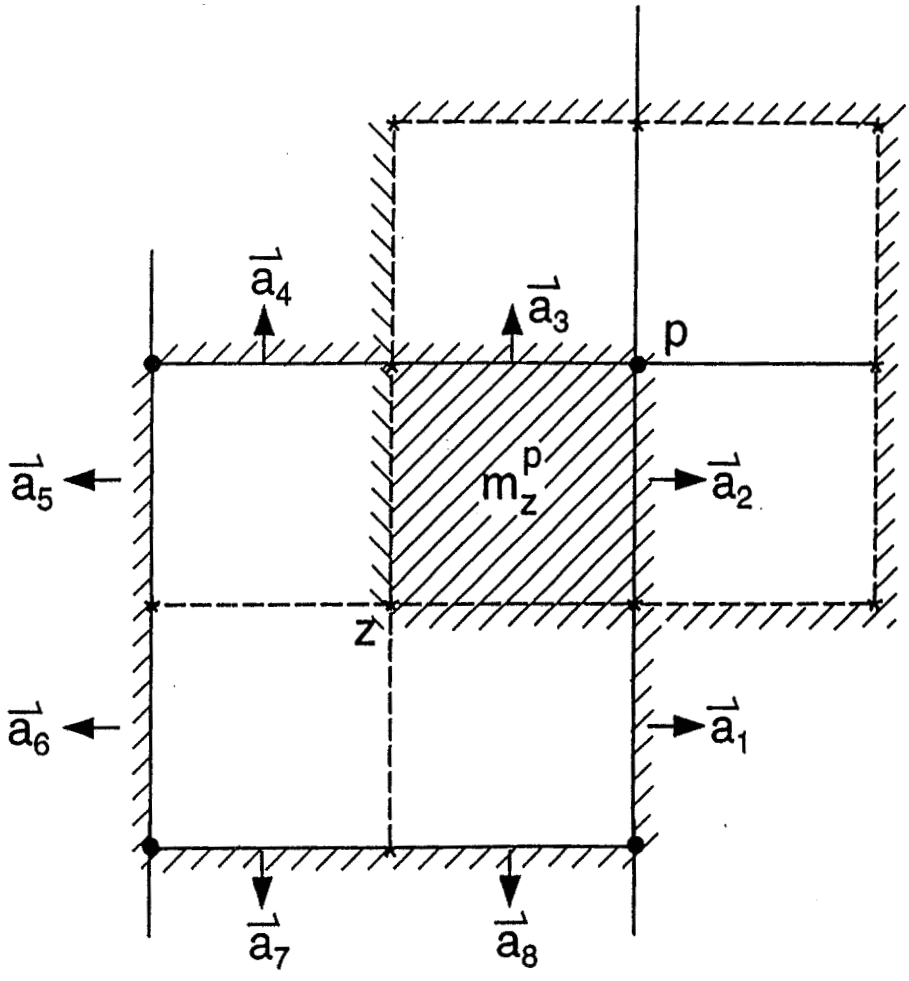

Figure(1) Quadrilateral zone and median mesh for defining corner mass m_z^p. Hatched lines denote Lagrangian boundaries of coordinate-line (solid) and median (dashed) mesh. $\vec{a}_i$ are outward normals to coordinate-line mesh.