THE GHOST FLUID METHOD FOR NUMERICAL TREATMENT OF DISCONTINUITIES AND INTERFACES

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Abstract.

The Ghost Fluid Method (GFM) has recently been developed to handle interfaces in a robust and efficient fashion leading to a general class of "boundary condition capturing" techniques based on the identification of "continuous" and "discontinuous" variables and the subsequent treatment of these variables to allow seamless finite differencing across the interface.

1. Introduction

The most commonly used computational methods for interfaces are front tracking, volume of fluid, and level set methods. While each of these methods have well known strengths and weaknesses, only the level set method will be addressed in this paper, since the GFM has been developed using level set techniques for the interface. However, it should be noted that the GFM is not a level set specific method and could be extended to front tracking or volume of fluid formulations in a straightforward way. Level Set methods were first presented in (Osher and Sethian, 1988) where the time dependent level set equation

$$\phi_t + \vec{W} \cdot \nabla \phi = 0 \tag{1}$$

was used to keep track of the interface location as the set of points where $\phi = 0$. Although ϕ is initialized as a smooth signed distance function, it usually loses this desirable property as the interface deforms under the velocity \vec{W} making it necessary to apply reinitialization in order to keep $|\nabla \phi| \approx 1$ (Sussman et. al., 1994). Another useful equation

$$I_{\tau} + \vec{N} \cdot \nabla I = 0 \tag{2}$$

can be used to extrapolate the quantity I in the normal direction (Fedkiw et. al., 1999a).

2. Conservation

Traditionally, Eulerian based numerical methods for compressible flow are based on the Lax-Wendroff Theorem (Lax and Wendroff, 1960) which dictates that numerical methods should be fully conservative, and it is well known that nonconservative methods produce shocks with incorrect speeds and strengths. However, (Karni, 1996) advocates nonconservative form at contact discontinuities which are lower dimensional sets (e.g. one dimensional in a two dimensional calculation) that move with the local fluid velocity. In (Karni, 1996), full conservation was applied away from interfaces and a nonconservative method was applied near interfaces without adversely effecting the shock speeds or strengths. Since shocks do not move at the local interface velocity, any portion of a shock is only in contact with an interface, and thus the nonconservative method, on a set of measure zero in space and time minimizing the accumulation of errors.

While it is true that others have used nonconservative discretizations, there is no doubt that the work in (Karni, 1996) is responsible for markedly increasing their popularity in the shock capturing community where traditionally schemes were thought to require conservation at all cost. In part, this is because (Karni, 1996) identified and fixed large numerical oscillations introduced at interfaces by the fully conservative scheme presented in (Mulder et. al., 1992). It is interesting to note that many front tracking and volume of fluid schemes are actually nonconservative, i.e. they do not satisfy the strict flux differencing conservation form usually thought to be required by the Lax-Wendroff Theorem. In this sense, many of these schemes share similar properties with the scheme in (Karni, 1996). For example, consider the front tracking approach in (Pember et. al., 1995) where a high order Godonuv method is used to obtain a nonconservative update near the tracked interface and a fully conservative update away from the tracked interface. All flow features including shock speeds and strengths as well as the speed of the tracked front are correctly determined as is ensured by the solutions of the appropriate Riemann problems. Note that the authors go one step further and correct the lack of conservation at the interface using a redistribution procedure (Chern and Colella, 1987) which is presumably not necessary for obtaining a grid resolved solution, but is only used to maintain exact conservation. In fact, the nature of this redistribution procedure does not allow strict application of the Lax-Wendroff Theorem, and one has to believe that the correct solutions are obtained because the numerical method is fully conservative except at the lower dimensional tracked interface which is updated correctly based on solutions of the appropriate Riemann problems. Similar loss of exact conservation occurs in volume of fluid methods where nonphysical overshoots may occur in the volume fraction equation (Puckett et. al., 1997). These overshoots can be ignored violating conservation, or redistributed in a manner similar to (Chern and Colella, 1987) to preserve exact conservation.

3. Isobaric Fix

The well known "overheating effect" occurs when a shock reflects off of a solid wall boundary causing overshoots in temperature and density, while pressure and velocity remain constant. In one spatial dimension, a solid wall boundary condition can be applied with the aid of ghost cells by constructing a symmetric pressure and density reflection and an asymmetric normal velocity reflection about the solid wall. Then a shock wave impinging on the wall will collide with a shock in the ghost cells that has equal strength traveling in the opposite direction producing the desired shock reflection. In (Menikoff, 1994) and (Noh, 1978), the authors showed that overheating errors are a symptom of smeared out shock profiles and that sharper shocks usually produce less overheating. In addition, they showed that the pressure and velocity equilibrate quickly, while errors in the temperature and density persist. In order to dissipate these errors in temperature and density, (Noh, 1978) proposed adding artificial heat conduction to the numerical method in a form similar to artificial viscosity. Later, (Donat and Marquina, 1996) proposed a flux splitting method with a built in heat conduction mechanism that dissipates these errors throughout the fluid.

At this point, it is instructive to consider the one dimensional Euler equations and the associated Rankine-Hugoniot jump conditions for a discontinuity moving at speed D. Since a solid wall moves at the local flow velocity, $D = V_N$ and Rankine-Hugoniot jump conditions of $[V_N] = 0$, [p] = 0, and 0 = 0 describe the relationship between the external flowfield and the internal one, i.e. both the normal velocity and the pressure must be continuous across the solid wall boundary extending into the ghost cells. Since these jump conditions are inherently part of the equations and thus part of any consistent numerical method, jumps in pressure and velocity are hard to maintain for any duration of time at a solid wall boundary, i.e. jumps between the fluid values and the ghost cell values are quickly dissipated. In this sense, one can think of pressure and velocity equilibration at a solid wall boundary as an intrinsic action of the boundary conditions. Note that there is no such condition for the temperature or the density. In the case of a complete equation of state (Davis, 1985), only one variable in the linearly degenerate field need be defined and all other variables can be determined from the equation of state relations. In this sense, one can state that there is no boundary condition for the linearly degenerate field as is emphasized by the trivially satisfied jump condition 0 = 0. Since a solid wall boundary is an initial boundary value problem, the value of the temperature at the wall must come from initial data as one can see from

$$S_t + \vec{V} \cdot \nabla S = 0 \tag{3}$$

which states that entropy is advected along streamlines of the fluid implying that the entropy near the wall stays near the wall since the wall moves with the local fluid velocity. We stress that this equation is only valid for smooth flow and is not true for streamlines that cross shock waves, i.e. entropy jumps across a shock wave. However, shock waves do not move at the same speed as solid wall boundaries so this equation is true near the wall most of time, i.e. except for a lower dimensional subset of space and time.

In (Fedkiw et. al., 1999c), equation 3 was used to develop the Isobaric Fix which is a boundary condition type of treatment for the linearly degenerate field at a solid wall boundary. The Isobaric Fix modifies the linearly degenerate field at a solid wall without changing the values of the pressure or the normal velocity. Noting that entropy is advected along streamlines and that streamlines are continuous, the entropy errors at the wall are repaired using new values of entropy extrapolated from the surrounding flow. For example, replacing the entropy at the wall with the entropy of the neighboring cell gives a first order accurate value of the entropy at the wall for smooth entropy profiles. Higher order accurate extrapolation can be used as well, but this has been found to be quite dangerous in practice due to the presence of discontinuous shock waves that cause large overshoots when extrapolating. In multiple spatial dimensions, the solid wall can be represented as the zero level of a level set function and moved rigidly using equation 1 where \vec{W} is the spatially constant wall velocity or deformed with equation 1 and a spatially varying \vec{W} . Then the Isobaric Fix can be applied using equation 2 with I = S.

4. Ghost Fluid Method

Similar to a solid wall boundary, a level set function can be used to track a contact discontinuity as the set of points where $\phi=0$ separating two different fluids that each satisfy the Euler equations with different equations of state. Since the equation of state properties are discontinuous across the interface, the discretization techniques are employed in a similar fashion as for a solid wall boundary, except that they are applied twice, i.e. once for each fluid. Conceptually, each grid point corresponds to one fluid or the other and ghost cells can be defined at every point in the computational

domain so that each grid point contains the mass, momentum, and energy for the real fluid that exists at that point (according to the sign of the level set function) and a ghost mass, momentum, and energy for the other fluid that does not really exist at that grid point (the fluid from the other side of the interface). Once the ghost cells are defined, standard one phase numerical methods can be used on the entire domain for each fluid, i.e. we now have two separate single fluid problems. After each fluid is advanced in time, the level set function is updated using equation 1 with $\vec{W} = \vec{V}$ (the local fluid velocity), and the sign of the level set function is used to determine the appropriate real fluid values at each grid point. Note that ghost cells are defined everywhere for exposition, but only a band of 3 to 5 ghost cells is actually used in practice.

Since contact discontinuities move at the local fluid velocity, the Rankine-Hugoniot jump conditions for a contact discontinuity are the same as those for a solid wall boundary, i.e. $[V_N] = 0$, [p] = 0, and 0 = 0. In multiple spatial dimensions, the 0 = 0 jump condition is repeated since the tangential velocities are also governed by the linearly degenerate field, e.g. in three spatial dimensions one can only determine the pressure and normal velocities from the boundary conditions, while the entropy and both tangential velocities remain undetermined. Note that in the case of the full viscous Navier-Stokes equations, the physical viscosity imposes continuity of the tangential velocities, and thermal conductivity imposes continuity of the temperature. Since certain properties are discontinuous across the interface, one should be careful when applying finite difference methods across the interface, since differencing discontinuous quantities leads erroneously to terms of the form $\frac{1}{\triangle x}$ that increase without bound as the grid is refined. Therefore, the layer of ghost cells should be introduced so that there is continuity with the neighboring fluid that needs to be discretized. For variables that are already continuous across the interface, e.g. pressure and normal velocity, the ghost fluid values can be set equal to the real fluid values at each grid point implicitly capturing the correct interface values of these variables. This is the key mechanism in *coupling* the two distinct sets of Euler equations. On the other hand, the discontinuous variables move with the speed of the interface (see equation 3), and information in these variables does not cross the interface and is not coupled to the corresponding information on the other side of the interface. Moreover, in order to avoid numerical smearing or spurious oscillations these discontinuous variables should not be nonphysically coupled together or forced to be continuous across the interface. The most obvious way of defining the discontinuous variables in the ghost cells is by extrapolating that information from the neighboring real fluid nodes, e.g. the entropy can be extrapolated into the ghost cells using equation 2 in exactly the same way as it was when applying the Isobaric Fix producing a continuous entropy profile. Since entropy is characteristic of the equation of state information and the fluid itself, we denoted this method the Ghost Fluid Method (Fedkiw et. al., 1999a), i.e. ghost cells that are physically located in one fluid are filled with entropy from the neighboring fluid changing the kind of fluid in these cells without changing the way these cells behave, i.e. without changing the pressure and normal velocity. Note that, similar to the Isobaric Fix, one does not have to deal directly with the entropy but can choose any variable in the linearly degenerate field, e.g. density or temperature. Since the tangential velocities are discontinuous as well, a similar extrapolation procedure is used to treat these variables making use of a basis free projection method (Fedkiw et. al., 1999a).

5. Other Discontinuities

For a simple contact discontinuity, the variables were separated into two sets based on their continuity across the interface. The continuous variables were copied into the ghost fluid in a node by node fashion capturing the correct interface values, while the discontinuous variables were extrapolated in a one-sided fashion to avoid errors due to numerical dissipation. In order to apply this idea to a general interface moving at speed D in the normal direction, one needs to correctly determine the continuous and discontinuous variables for a general interface problem. For example, consider a shock wave where all variables are discontinuous, and extrapolation of all variables for both the pre-shock and post-shock fluids obviously gives the wrong answer since the physical coupling is ignored. We state, "For each degree of freedom that is coupled across a discontinuity, one can define a variable which is continuous across the discontinuity, and all remaining degrees of freedom can be expressed as discontinuous variables which can be extrapolated across the interface in a one-sided fashion." as the key to extending the GFM. In the case of the Euler equations, conservation of mass, momentum, and energy can be applied to any discontinuity in order to abstract continuous variables, i.e. the Rankine-Hugoniot jump conditions always dictate the coupling between the pre-discontinuity and post-discontinuity fluids. In (Fedkiw et. al., 1999b), the Rankine-Hugoniot relations were used in three spatial dimensions to define F_{ρ} , $F_{\rho V_N}$, $\vec{F}_{\rho V_T}$, and F_E as continuous variables across a discontinuity which has speed $D \neq \vec{V_N}$, i.e. when the discontinuity is not a contact discontinuity. This allowed us to develop a GFM that implicitly captures the interface values of these continuous quantities at shocks, detonations, and deflagrations, i.e. the method implicitly captures the Rankine-Hugoniot jump conditions without numerical smearing.

When the GFM is used for general discontinuities, one needs to accurately find the interface speed D for equation 1 with W = DN. For shock waves and detonation waves, D can be found by solving an appropriate Riemann problem in a node by node fashion (Fedkiw et. al., 1999b). In fact, there is no reason one cannot solve a Riemann problem in the case of a contact discontinuity as well using $\vec{W} = D\vec{N}$ in equation 1 as opposed to $\vec{W} = \vec{V}$ (the less accurate local fluid velocity) (Fedkiw et. al., 1999b). Note that a combination of ghost cells and Riemann problems is commonly used in front tracking algorithms, see e.g. (Glimm et. al., 1980) and (Glimm et. al., 1999) where a Riemann problem is solved at the interface and the results are extrapolated into the ghost cells. The difference between the GFM and typical front tracking is in the order of operations, i.e. front tracking algorithms first solve a Riemann problem and then extrapolate while the GFM extrapolates first and then solves the Riemann problem in a node by node fashion removing some of the complications due to geometry. For a deflagration wave, the Riemann problem is not well posed unless the speed of the deflagration, i.e. D, is already given. Luckily, the G-equation for flame discontinuities (first proposed in (Markstein, 1964)) represents a flame front as a discontinuity in the same fashion as the level set method so that one can easily consult the abundant literature on the G-equation to obtain deflagration speeds.

6. Incompressible Flow

In multiphase incompressible flow calculations, a variable coefficient Poisson equation needs to be solved since the density is usually different (although constant) in each phase. This equation is not straightforward to solve especially when $[p] \neq 0$ which is typical for any multiphase flow problem where the viscosity jumps across the interface or surface tension is present. The most notable method for solving the Poisson equation is probably the "immersed boundary" method (Peskin, 1977) which uses a δ -function formulation to smear out the solution on a thin finite band about the interface. However, this numerical smearing has an adverse effect on the solution forcing continuity at the interface regardless of the appropriate interface boundary conditions, i.e. the nonzero jump in the pressure is not accurately represented. This failing has been overcome by a number of authors who solve the Poisson equation with [p] = 0 and then add new source terms to the momentum equations, see e.g. (Brackbill et. al., 1992), (Unverdi and Tryggvason, 1992) and (Sussman et. al., 1994). In the interest of solving the Navier-Stokes equations directly, i.e. without the addition of source terms, a new GFM was designed for the variable coefficient Poisson equation (Liu et. al., 2000) allowing one to solve this equation with both [p] and $[\frac{p_n}{a}]$ as given nonzero jumps, and ρ discontinuous. This new method used the given jump conditions to define continuous variables for the finite differencing similar to the way that the Rankine-Hugoniot jump conditions were used for multiphase compressible flow. It is notable that the resulting system of linear equations is completely symmetric allowing for straightforward application of standard linear system solvers. This new numerical method does not suffer from the numerical smearing prevalent in the "immersed boundary" method and was used to solve the multiphase Navier-Stokes equations in (Kang et. al., 2000) without the need for additional source terms.

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