NUMERICAL SIMULATION OF 2-D TWO-PHASE FLOWS WITH INTERFACE

S. KOKH
DRN/DMT/SERMA,
CEA Saclay, 91191 Gif-sur-Yvette, France.

AND

G. ALLAIRE
Laboratoire d'Analyse Numérique,
Université Paris-VI, 75252 Paris Cedex 5, France.

Abstract

This paper is devoted to the direct numerical simulation of compressible two-phase flows, *i.e.* including material interfaces, in an Eulerian framework. Eulerian methods, such as Volume Of Fluid, are easy to handle but suffer from numerical diffusion which spreads out the precise localization of the interface. We discuss some remedies to this loss of accuracy.

1. Introduction

Modelization and simulation of bifluid and diphasic flows have become of increasing interest among the computational fluid dynamic community. So-called direct simulation, on the contrary of average models, involves the description of the interface between fluids which is a discontinuity surface for the material properties. We propose a model for compressible two-phase flows. The dynamical aspect of the problem is handled by the compressible Euler equations, written for the overall mixture, while the phase interface is captured on an Eulerian mesh. An extra equation is therefore added to the Euler system in order to advect values of a color function ψ according to the fluids motion. This type of systems has been studied by Abgrall (Abgrall R, 1988) and Karni (Karni S, 1996). This approach provides key features such as no extra complexity in dealing with "high-dimensional" problems, easy handling of drastic topological changes or complex topol-

ogy of the interface between the two phases. The other side of the coin is a lack of accuracy for the interface description in contrast to methods involving interface reconstruction such as Front Tracking. In fact, numerical diffusion tends to thicken the interface into a transition zone which is no longer a sharp discontinuity between the media. We focus on the numerical diffusion problem near contact discontinuities. Simple observations for a single transport equation lead us to propose various processes for improving the accuracy of the interface description while preserving the ease-of-use of interface capturing methods.

2. Bifluid solver: model and numerical treatment

The model used here follows the line of Abgrall in (Abgrall R, 1988). The motion of the fluids is here driven by the compressible Euler equations (1)–(3). It is supplied by the color function transport equation (4) and an equation of state (EOS) that closes the system. For the sake of simplicity we expose the method in the case of a perfect gas EOS, despite the process is still valid for more general laws such as Stiffened Gas. Numerical diffusion implies that some cells do contain both species. Upon an isothermal assumption, Abgrall showed how to construct an EOS of the form (5) in order to deal with the mixture zone and which reduces to the usual perfect gas EOS in pure fluid areas.

$$\partial_t \rho + \mathrm{div}(\rho \vec{\mathrm{u}}) = 0, \tag{1}$$

$$\partial_t \rho \vec{u} + \mathrm{div}(\rho \vec{\mathrm{u}} \otimes \vec{\mathrm{u}}) + \overrightarrow{\mathrm{grad}}\mathrm{p} = \vec{F}, \tag{2}$$

$$\partial_t \rho e + \mathrm{div}\Big[(\rho \mathrm{e} + \mathrm{p})\vec{\mathrm{u}}\Big] = Q, \tag{3}$$

$$\partial_t \psi + \vec{u} \cdot \overrightarrow{\mathrm{grad}}\psi = 0, \tag{4}$$

$$p = p(\rho_1, \rho_2, \rho(e - |\vec{u}|^2/2)). \tag{5}$$

$\vec{F} = (F_x, F_y)$ and Q are source terms such as gravity, viscosity, surface tension, and thermal diffusion.

We briefly describe the numerical method used to implement the model. The Euler system is solved thanks to a Roe-type scheme (Roe P L, 1981), as done in (Abgrall R, 1988) for the variables $(\rho, \rho\vec{u}, \rho e)$. As mentioned by Karni in (Karni S, 1994), conservative schemes have difficulties to describe accurately the pressure near the interface generating spurious oscillations. To remedy this drawback, Abgrall proposes in (Abgrall R, 1988) to judiciously choose $\psi = 1/\kappa$ (κ being the Grünsein constant) as color function and derives a discretization of (4) that preserves numerical contact discontinuities. Gravity is treated as a centered source term, viscosity and thermal diffusion are discretized by standard finite differences while we use the continuous surface tension model of (Brackbill J, Kothe D and Zemach C,

1992) for the interfacial tension. Second order accuracy in space is reached thanks to a MUSCL method with a minmod limiter. As for second order in time, we use a two-point Runge-Kutta method. Unfortunately even second order accuracy in space and time cannot help to decrease numerical diffusion for long. Indeed even if the numerical scheme succeeds in picturing the behaviour of the system, it may happen that an entire fluid component just disappears into the mixture zone. Let us emphasize that mixture zones do not have necessarily any real physical sense. Furthermore it may also become very difficult to describe jumps of variables across the interface which are of high interest for modeling physical process such as mass transfer due to phase changes. In the sequel we propose various methods to maintain the sharpness of contact discontinuities (material interfaces).

3. The transport equation model

We focus in this section on the specific problem of numerical diffusion of finite difference schemes near contact discontinuities. To begin with, let us underline that the structure which drives the contact discontinuity is a linearly degenerated field. Harten in (Harten A, 1978) enlightens the behavior of a discontinuity line advected by such field and approximated by a classical numerical scheme. The width of the numerical diffusion will inexorably grows as the number of time steps increases, on the contrary to shocks driven by genuinely non-linear fields which are enclosed in a viscous profile. The most simple equation that can mimic the critical behavior of such fields is a simple linear transport equation at constant speed. Let $u(t,x)$ be the solution of

$$\partial_t u + c\partial_x u = 0, \quad \forall x \in \mathbb{R}, \quad \forall t > 0 \tag{6}$$

with the initial condition $u(0,x) = u_0(x)$, c being a constant velocity. The exact solution is $u(t,x) = u_0(x-ct)$. We are interested in the case where u_0 is a step function, and study the numerical diffusion associated to a given numerical scheme. We first recall the influence of order accuracy upon numerical diffusion. All computations are done with an upwind scheme for $c = 1$ on a segment $\mathrm{I} = [0,1]$, meshed by 1000 regular cells, with periodic boundary conditions and $u_0 = \mathbb{1}_{[1/4,3/4]}$. Second order in space and time are respectively implemented via a MUSCL method with minmod limiter and a two-points Runge-Kutta method. As expected, for the first order scheme the L^1-norm of the error grows like $\sqrt{n}$, where n is the number of time steps. When switching to second order in space, the error L^1-norm stops increasing after a few time steps. However, for both time and space second order, the numerical diffusion of the scheme grows again unbounded. Thus, second order in space with first order in time would be quite satisfactory,

but in many cases second order in time is necessary to stabilize numerical oscillations. For example, the simple computation of the hydrostatic pressure establishment upon the influence of gravity in a single fluid turns out to be impossible due to instabilities. Such simple examples motivate our study of procedures to bound this extra diffusion. The level set method provides a way to exactly control the thickness of the interface. It uses instead of the discontinuous color function a continuous function initialized as the signed distance to the interface as exposed in (Sethian J, 1996) or (Mulder S, Osher S and Sethian J, 1992). This function is frequently reinitialized during the computation by solving a suitable Hamilton-Jacobi equation as mentioned in (Sethian J, 1996) and (Sussman M, Smereka P and Osher S, 1994). Here, staying in the framework of the VOF method, we propose to add source terms in order to straighten up the front.

4. Sharpening source terms

To begin with, we introduce in (6) a source term $P(u) = \eta u(1-u)(u-1/2)$ where η is a real parameter. This source term does not modify the exact solution of this equation since it can only take the values 0 or 1. However, in the discrete problem it will act as a "repelling force" on the approximate solution. Values above 1/2 will be pushed towards 1, while those below will get closer to 0. Two numerical implementations of this source term are possible. First of all, it can simply be added into the discretized equation as a centered source term. Alternatively, a splitting-like method can be chosen: the classical upwind scheme resolution is stopped after N time steps then the approximated solution u^N at instant N is sharpened by solving $\partial_s v = P(v)$ with initial condition $v(0,x) = u^N$ until it reaches a steady state (s is an artificial time variable). Fortunately, there exists explicit solutions of this ODE, thus no new extra computational work is required. A second type of source term can be obtained by changing the constant η into a variable quantity $\eta\partial_x u$, which yields $Q(u, \partial_x u) = \eta u(1-u)(u-1/2)\partial_x u$. In this case, equation (6) can also be rewritten

$$\partial_t u + \partial_x[cu + (\eta/4)u^2(1-u)^2] = 0$$

Actually, this appears to be a flux modification of (6) which fits into the framework of the artificial compression method developed by Harten in (Harten A, 1978). Figure 1 displays a comparison of the growth for the L^1-error between the different methods. Accuracy gain is obvious for the first order method as the L^1-error stops growing after a few time steps. While for second order in space only the process doesn't show real improvement, it succeeds in slowing down the error growth second order is applied to both space and time. The efficiency of such sharpening process can be quantified

by studying the equivalent equation of the numerical scheme. Indeed, for the case of an upwind first order scheme, a viscosity profile (having the shape of a tanh function) can be explicitly computed for the initial value problem (6).

5. Application to the bifluid model

The sharpening process described earlier is applied to the advection equation for $\psi = 1/\kappa$ in system (1)–(5) introducing the source term

$$Q(\psi) = -\eta(\psi - \psi_1)(\psi - \psi_2)(\psi - (\psi_1 + \psi_2)/2)$$

in the scheme as a centered source term. Figure 2 shows the effect of sharpening ($\eta = 0.2$) on the computing of a shock into an helium bubble surrounded by air (Abgrall R, 1996) on a $1\text{m} \times 1\text{m}$ mesh discretized in 100×100 regular cells. Notice that the other variables seem to be unaffected by the sharpening source term.

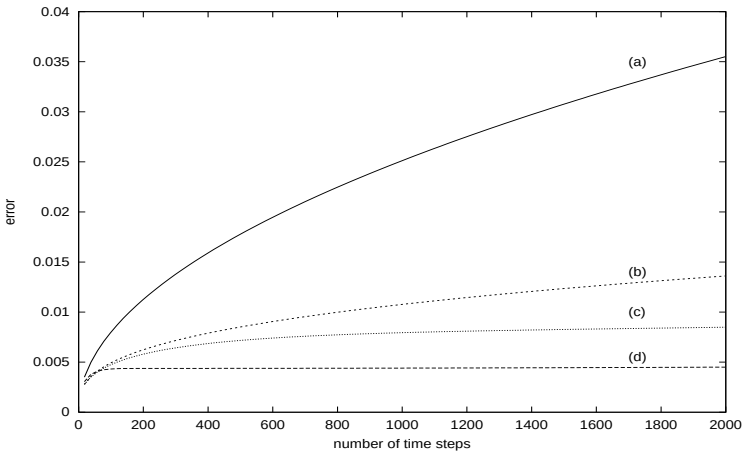

Figure 1. L^1-error for an impulse advection after 2000 time steps, (a): order one, (b):order 2 scheme in both time and space, (c) order 2 scheme in both time and space with centered source term correction for $\eta = 5 \times 10^{-3}$, (d): order one with centered source term correction for $\eta = 0.1$.

6. Conclusion and perspectives

We have developed a simple method for sharpening the advection of discontinuities in finite differences numerical schemes. This method is easy to use and adds no extra complexity when dealing with 2-D and 3-D problems. The primary goal is to improve the localization of material interfaces in compressible two-phase flow simulation. Important variables, such as pressure,

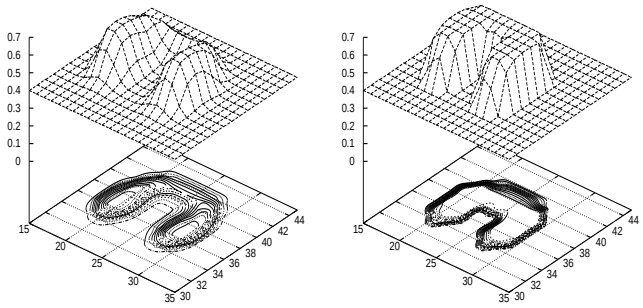

Figure 2. profile for κ, without sharpening on the left, with sharpening on the right, at instant $t = 0.35$s

density and velocity, do not seem to be noticeably affected by this sharpening. We hope to be able to derive new further estimates for second order schemes in both time and space. Concerning applications to two-phase flows with phase change at the interface, we have obtained preliminary results by adding a kinetic relation to determine the interface velocity as described in (Truskinowsky L, 1991). Alternate advection schemes for the color function such as level set and characteristic methods have been implemented, while the extension of the model to stiffened gas is in progress. This will be the topic of future reports.

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