Anti-diffusion Interface Sharpening Technique for Two-Phase Compressible Flow Simulations

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1 Introduction

Shock waves in two-phase compressible flows are a fundamental topic in science and engineering. To better understand instability phenomena that are important for the evolution of such flows, basic configurations such as shock-bubble interactions in two-phase compressible flows are considered to investigate the Richtmyer-Meshkov instability and Rayleigh-Taylor instability. Flows of this type are present in many engineering applications including supersonic mixing and combustion systems and extra-corporeal shock-wave lithotripsy.

Numerical models of two-phase compressible flows play a significant role in the study of the topic as they provide the access to flow regimes and quantities which cannot be studied and obtained analytically and experimentally. The main numerical methods for two-phase compressible flow simulations are the level-set methods [1], the volume-of-fluid (VOF) methods [2], and front-tracking methods [12].

The VOF volume-capturing method possesses the advantage of exact conservation properties, but suffers from numerical diffusion which causes two-fluid interfaces to smear. Specific numerical schemes to suppress or counter-act the numerical diffusion, and to maintain the interface sharpness in the course of simulations are thus desirable for VOF methods. Previous works include the interface compression technique by [9], and the anti-diffusive numerical scheme based on a limited downwind strategy [5].

In this paper, we propose an interface sharpening technique for two-phase compressible flow simulations. The idea is to solve an anti-diffusion equation for counter-acting the numerical diffusion. The technique has been developed and verified for two-phase incompressible flow simulations [10]. It is the objective of this paper to present the key concepts and numerical results of the application of the technique to two-phase compressible flow simulations.

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2 Governing Equations

We consider the Euler equations assuming a single velocity and pressure equilibrium. The two phases are represented by the volume fractions, where the formulation of the volume-fraction equations of [2] is adopted. The volume-fraction equation formulation has been extensively studied by [6] for simulations with ideal-gas equation of state (EOS) and Mie-Grüneisen EOS, and serves as the governing equations for a computational study for shock-bubble interactions by [7]. With two mass conservation equations, one momentum conservation equation and one energy conservation equation a six-equation model is obtained as follows:

$$\frac{\partial \alpha}{\partial t} + \nabla \cdot \alpha \mathbf{u} = \alpha \frac{\overline{K}_S}{K_S^\alpha} \nabla \cdot \mathbf{u} \quad , \tag{1}$$

$$\frac{\partial \beta}{\partial t} + \nabla \cdot \beta \mathbf{u} = \beta \frac{\overline{K}_S}{K_S^\beta} \nabla \cdot \mathbf{u} \quad , \tag{2}$$

$$\frac{\partial \alpha \rho^\alpha}{\partial t} + \nabla \cdot \alpha \rho^\alpha \mathbf{u} = 0 \quad , \tag{3}$$

$$\frac{\partial \beta \rho^\beta}{\partial t} + \nabla \cdot \beta \rho^\beta \mathbf{u} = 0 \quad . \tag{4}$$

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot \rho \mathbf{u}\mathbf{u} + \nabla p = 0 \quad , \tag{5}$$

$$\frac{\partial E}{\partial t} + \nabla \cdot (E + p)\mathbf{u} = 0 \quad , \tag{6}$$

where α and β are the volume fractions of the two phases respectively and $\alpha + \beta = 1$, t is the time, $\mathbf{u}$ is the velocity, $\overline{K}_S$ is the mixture bulk modulus, K_S^α and K_S^β are the phase bulk modului, ρ^α and ρ^β are the phase densities, p is the pressure and E is the total energy.

3 Numerical Methods

3.1 Riemann Solver

The HLL Riemann solver [13] is adopted for calculating the numerical flux at cell face, $\mathbf{F}_{HLL}$,

$$\mathbf{F}_{HLL} = \begin{cases} \mathbf{F}_L & \text{if } 0 \le S_L, \\ \frac{S_R \mathbf{F}_L - S_L \mathbf{F}_R + S_L S_R (\mathbf{U}_R - \mathbf{U}_L)}{S_R - S_L} & \text{if } S_L \le 0 \le S_R, \\ \mathbf{F}_R & \text{if } 0 \ge S_R, \end{cases} \quad , \tag{7}$$

where $\mathbf{U}$ is the cell-averaged conserved variable, $\mathbf{F}$ is the cell-average flux, S is the bound of the fastest signal velocity, and the subscripts L and R denote the two sides of the cell face.

3.2 Anti-diffusion Interface Sharpening

The idea of sharpening the two-fluid interface is to provide a correction algorithm which can be applied as post-processing to the volume-fraction field after each time step. For such, an anti-diffusion equation, i.e. a diffusion equation with a positive diffusion coefficient, is solved to counter-act the numerical diffusion

$$\frac{\partial \alpha}{\partial \tau} = -\nabla \cdot (D \nabla \alpha) \quad , \tag{8}$$

where $D > 0$ is an anti-diffusion coefficient and τ is a pseudo time.

A specified discretization scheme is employed to ensure the numerical stability and volume-fraction boundedness in solving the anti-diffusion equation. The solution procedure is described in [10]. First, the limited cell-averaged value of the gradient of α, $\overline{\nabla \alpha}$, is obtained by the regularization based on a minmod limiter. Then, the anti-diffusion flux for α, F^{α}_{AD}, at the cell face between cell P and cell N is obtained by:

$$F^{\alpha}_{AD} = \begin{cases} -|D| \overline{(\nabla \alpha)_P} \cdot \mathbf{S} & \text{if } |\overline{(\nabla \alpha)_P}| \leq |\overline{(\nabla \alpha)_N}| \\ -|D| \overline{(\nabla \alpha)_N} \cdot \mathbf{S} & \text{if } |\overline{(\nabla \alpha)_N}| < |\overline{(\nabla \alpha)_P}| \end{cases} , \tag{9}$$

where $|\overline{(\nabla \alpha)_P}|$ and $|\overline{(\nabla \alpha)_N}|$ are the respective limited cell-averaged value of the gradient in cell P and cell N, $\mathbf{S}$ is the cell surface area vector.

The right-hand-side of eq. (8) is calculated by

$$\overline{\nabla \cdot (-|D| (\nabla \alpha))} = \frac{\sum_{cf} \left(F^{\alpha}_{AD} \right)}{V} \quad , \tag{10}$$

where $\sum_{cf}$ denotes the summation over all cell faces, V is the cell volume.

The volume fraction is advanced in pseudo time by an explicit Euler scheme:

$$\alpha^{AD} = \alpha + \overline{\nabla \cdot (-|D| (\nabla \alpha))} \Delta \tau \quad , \tag{11}$$

with the time step limit on pseudo time, $\Delta \tau$

$$\Delta \tau = \frac{1}{4} \frac{(\Delta x_{min})^2}{|D|} \quad . \tag{12}$$

α^{AD} is the sharpened volume fraction, Δx_{min} is the minimum cell width.

As the anti-diffusion equation is meant to counter-act the numerical diffusion resulted from the volume-fraction transport, the choice of D is based on the numerical

diffusion of the numerical scheme. Hence based on the formulation of the HLL Riemann solver D is chosen to be

$$D = \frac{S_L S_R (\alpha_R - \alpha_L)}{S_R - S_L} \quad . \tag{13}$$

The anti-diffusion equation can be solved repeatedly to attain an even sharper profile. A case- and grid- independent stopping criteria as detailed in [10] is employed to terminate the sharpening iterations.

After each time α is sharpened, all other flow variables in the governing equations are updated according to α^{AD} to ensure the consistency. Typically, only 1-2 sharpening iterations are sufficient in each time step.

4 Numerical Results

For all cases in the section the reconstruction of U_L and U_R is calculated by the van Leer MUSCL scheme. A third-order TVD Runge-Kutta method is employed for time integration. The time step for the governing equations is determined by the CFL requirement with a CFL number of 0.2.

4.1 Shock Tube Problem

The one-dimensional air-helium shock tube case of [4] is considered. The domain is defined as $[0,1]$ and discretized by 200 cells. The initial condition is

$$(\rho, u, p, \gamma) = \begin{cases} (1,0,1,1.4) & \text{if } 0 \leq x < 0.5 \\ (0.125,0,0.1,1.667) & \text{else} \end{cases} , \tag{14}$$

The results with and without the application of the anti-diffusion interface sharpening technique at $t = 0.15$ are shown in Fig. 1. By comparing the two results, one can see that the phase interface is better resolved, as can be seen from the reduced number of transition points in α, with the application of the anti-diffusion interface sharpening technique. The improved interface resolution also transfers to the other variables.

4.2 Shock-Bubble Interaction

The experimental case of a R22 cylinder in air hit by a shock wave at Mach number of 1.22 of [3] is considered. Corresponding to the reference literature, the simulation is treated as two-dimensional and the case set-up of [11] and the fluid parameters of [8] are adopted here. The domain is discretized by a Cartesian grid of

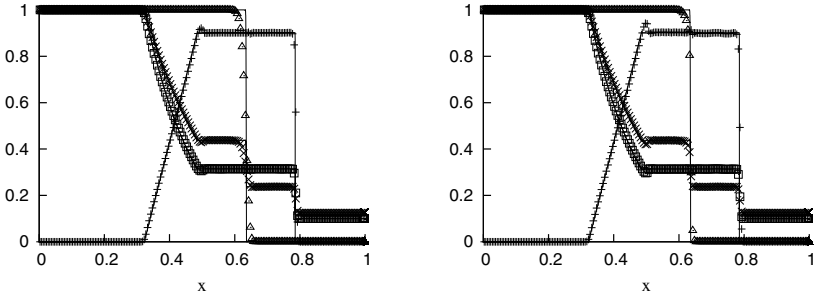

Fig. 1 Variables at $t = 0.15$ of the air-helium shock tube. '$\triangle$' denotes α, '$\times$' denotes ρ, '$+$' denotes $|\mathbf{u}|$, '$\square$' denotes p. Solid lines are the analytical solutions. Left: no interface sharpening; right: with interface sharpening.

$\Delta x/D = \Delta y/D = 0.005$, which is equivalent to a grid of a resolution of 200 cells across the bubble diameter.

The numerical Schlieren images, $|\nabla\rho|$, at $t = 187\mu s,\ 417\mu s$ after the shock impact are shown in Fig. 2. With the application of the interface sharpening technique the two-phase interface is better resolved while the large-scale structures remain consistent with the reference solution where no sharpening was applied, and with the reference literature [8]. More small-scale structures are recovered by the sharpening technique. The interface evolution of the high-resolution simulations computed on a grid of an effective resolution of $\sim$800 cells across the bubble diameter by an adaptive mesh refinement algorithm [8] are recovered by the simulations with interface sharpening on a mesh with about 16 times fewer grid points at the interface.

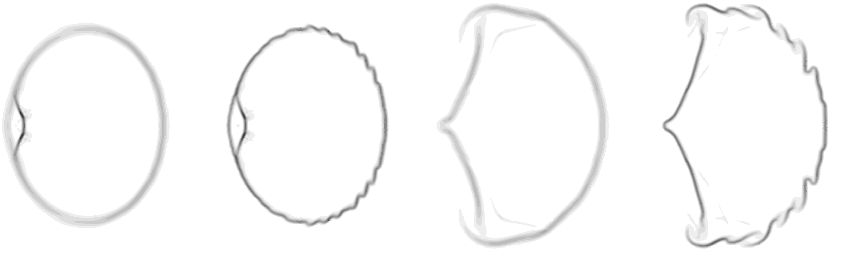

Fig. 2 Numerical Schlieren images, $|\nabla\rho|$, of the air-R22 shock-bubble interaction. From left to right: $t = 187\mu s$ (no interface sharpening), $t = 187\mu s$ (with interface sharpening), $t = 417\mu s$ (no interface sharpening), $t = 417\mu s$ (with interface sharpening).

5 Conclusion

In this paper an interface sharpening technique based on anti-diffusion is presented for two-phase compressible flow simulations. The technique possesses the advantage of being modular and applicable to any underlying VOF discretization schemes. The anti-diffusion flux to counter-act numerical diffusion is based on the anti-diffusion coefficient which is derived from the numerical scheme for the governing equations. The flow variables are updated consistently according to the sharpened volume fraction. Good agreement with experimental observation and simulation results from reference literature shows that more small-scale structures can be recovered by the interface sharpening technique.

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