A Numerical Scheme for Multi-component Flows

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Conservative schemes usually produce oscillations when used to solve multi-component flows. In order to overcome this problem numerous interface correction schemes have been developed. The present scheme is based on the interface correction scheme of Cocchi et. al. [3] with some improvements to their scheme in some cases. After each time step the two grid points that bound the interface are recalculated, eliminating pressure oscillations and density diffusion at the interface. This correction scheme can be applied to any type of conservation law solver. The interface itself was captured by using the level set approach and the flow field was computed with an upwind TVD scheme. This scheme was extended to two dimensional multi-component flows by using directional splitting. Some examples of planar shock wave in air interacting with a water cylinder are studied.

One of the main difficulties of shock capturing schemes such as TVD or ENO schemes is modeling multi-components flows. These difficulties are created as a result of the calculation of pressures from an equation of state based on the total energy in the gas. In multi-component flows, even when the densities and velocities are initially identical, the internal energy of each fluid will be different due to the difference of their specific heats ratios γ, and hence after one time step the energy diffusion across the interface will appear. It has been shown by Karni [5] when using γ which changes discontinuously across the interface, an incorrect value for the pressure will be calculated at the interface. In the next time step, a false velocity will be calculated since its derivation was based on the incorrect pressure value.

So far many researchers, Abgrall [1], Cocchi and Saurel [2], Cocchi, et al. [3], Jenny, et al. [4], Karni [5, 6], Shyue [7] proposed possible methods to overcome this problem. Most suggested use of a variety of quasi conservative schemes, e.g., Abgrall [1], Shyue [7], Karni [6]. In these schemes, the density change across the interface was not expressed sharply, but diffusely. When dealing with gas phase only, density diffusion might be acceptable, however when dealing with two phase flows such as gas and liquid phases accompanying large density change between these two phases, density diffusion across the interface is strictly unacceptable. No mixing takes place between gas/liquid interfaces except in very special cases. Numerical diffusions might result in unphysical densities at the interfaces. Therefore, a different method should be proposed to overcome this unphysical mixing. This method should eliminate pressure fluctuations at the interface and keep a discontinues density profile at the interface. Cocchi and Saurel [2] and Cocchi, et al. [3] managed to achieve those goals by employing a Godunov scheme coupled with a front tracking method. In order to correct the gird points near the interface that have been affected by diffusion their scheme uses results derived from the exact Riemann solver and grid points near the interface that have not been affected by diffusion for evaluating the grid points that bound the interface. Thereby correcting the density diffusion and pressure fluctuations at the interface. Therefore, the numerical density diffusion and pressure oscillations are removed and a sharp interface is maintained.

This paper improves the existing scheme by changing the interface tracking from front tracking method to a front capturing scheme the level set approach. A work employing the level set approach for gas dynamic problems was proposed by Mulder, Osher et al. [7]. Their method can be readily added to any schemes which are based on the approximate Riemann solver such as TVD or ENO schemes. It can handle the separation or merger of interfaces, whereas they are difficult to perform in the front tracking method. In addition, the front tracking method is more computationally demanding than the level set approach which requires only adding one more equation to the computational model.

The basic outline of the present scheme is to use an upwind TVD scheme with the level set approach for solving the flow field under study. After each iteration one should apply the correction step to the grid points on both sides of the interface. This is in a similar fashion to the scheme given by Cocchi, Saurel et al. [3]. For one dimensional problems this method resembles that of Cocchi, Saurel et al. [3]. However, in the present procedure the correction step has been improved for some cases and was modified to be used with the level set approach. Which is simpler in its application to two dimensional problems than the front tracking method.

2 Level set approach

Mulder, Osher et al. [7] have presented a TVD scheme incorporating the level set approach to track the interface between two gases. The level set approach is an interface capturing scheme based on level set functions. It can capture the interface between two grid points. Let the level set function ψ be defined as the distance between a grid point and the interface. $\psi=0$ designates the material interface. Where a positive value of ψ designates one material while a negative value of ψ designates the other material. Knowing the value of ψ the specific heats ratio can be defined as a function of the level set function. For example:

$$\gamma(\psi) = \begin{cases} \gamma, \psi > 0 & \text{gas} \\ n, \psi < 0 & \text{liquid} \end{cases}, \qquad (1)$$

The level set function propagates with the local fluid velocity. The numerical scheme solves the advection equation in non-conservative form in a similar method as that employed by Mulder, Osher et al. [7].

$$\psi_t + u\psi_x + v\psi_y = 0 \qquad (2)$$

The location of the interface can readily be found if the following equation is satisfied,

$$\psi_i \psi_{i+1} < 0, \qquad (3)$$

Where the interface is located between grid points i,i+1. Now that the use of the level set approach is explained, it will be incorporated into a system of hyperbolic conservation laws.

3 Governing equations

The governing equations for compressible inviscid flow in two-dimensions in conservation form are:

$$U_t + F_x + G_y = 0,$$

$$U = \begin{bmatrix} \rho \\ \rho u \\ \rho v \\ E \end{bmatrix}, \quad F(U) = \begin{bmatrix} \rho u \\ \rho u^2 + P \\ \rho uv \\ u(E+P) \end{bmatrix},$$

$$G(U) = \begin{bmatrix} \rho v \\ \rho uv \\ \rho v^2 + P \\ v(E+P) \end{bmatrix} \qquad (4)$$

where ρ, u, v, p and E are the density, velocity in x and y directions, pressure and total energy per unit of volume respectively. To these equations we add Eq. (2) to solve the level set function.

An integral part of every multi component scheme is the equation of state for the various fluid components. This is not a straight forward step since a different equation of state is needed for each fluid. It is an important part of any exact or approximate Riemann solver. To overcome this problem one can use the stiffened gas equation of state that can describe both the gas and the liquid. This equation of state has been previously employed in multi component flow simulations by [2, 3, 7, 9]. For example,

$$E = \frac{p + \gamma B}{(\gamma - 1)} + \frac{1}{2}\rho u^2, \qquad (5)$$

where B and γ are parameters for water $\gamma=7.415$ and B=296.3 MPa. When this equation is used for gases, B is set to zero and γ is equivalent to the specific heat ratio, for air $\gamma=1.4$. An approximate Riemann solver was modified to accommodate the stiffened gas equation of state. The proposed solver is based on that of Mulder, Osher et al. [7]. Further information about the numerical scheme can be found in [9].

4 Correction step

The interface correction step is based on that proposed by Cocchi, et al. [2], Cocchi and Saurel [3]. The main idea of this approach is that the two grid points just in front and behind the interface are recalculated in the corrector step; thus, a sharp density gradient is maintained. This is done by interpolating the results of the exact Riemann solver at the interface with results obtained from the grid points across the interface that have not been affected by diffusion. The flow chart of the correction step is shown in Fig. 1. There are two types of correction steps depending upon the location of the interface at time step n+1. The first is used when the interface remains within the same two grid points. The other is applied when the interface moves forwards or backwards, i.e., one of the two previous grid points is changed. For example at time step n the interface was located between grid point i and i+1, while at time step n+1 the interface is located between grid points i+1 and i+2. For each case a different interface correction step is utilized. An outline of the correction step is as follows: Firstly the location of the interface at time n between grid points i and i+1 is found

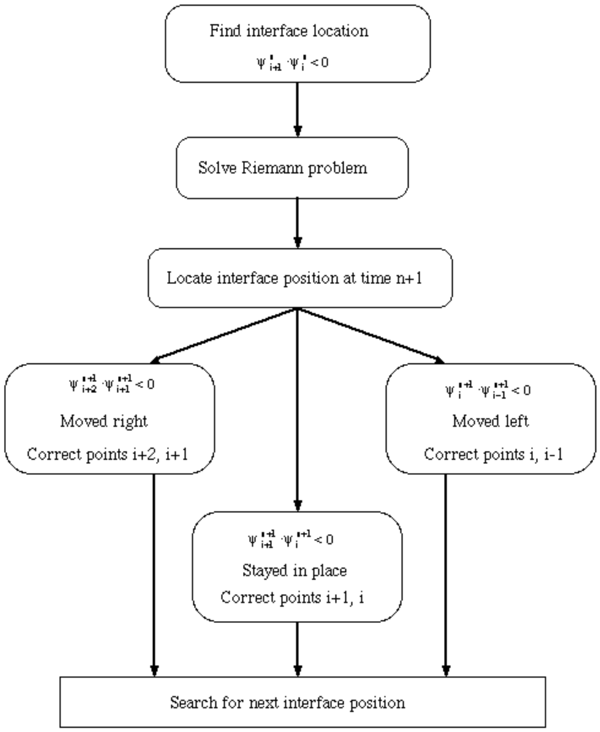

Fig. 1 Correction step flow chart

using Eq. (3). This procedure was described in Section 2, when $\psi^n_{i+1} \cdot \psi^n_i < 0$ the interface is located between the grid points i and i+1. The second step is to calculate an exact Riemann solver for grid points i and i+1 using the stiffened gas equation of state.

The correction step when the interface is still located between grid points i and i+1 shall be presented first. The interface location at the next time step n+1 can readily be found using Eq. (3) with the level set functions for time step n+1. Based on the level set function the interface location was calculated using the following equation,

$$x_{mi} = \frac{|\psi_i|}{|\psi_{i+1}| + |\psi_i|} \Delta x + x_i . \tag{6}$$

The interface location is needed to calculate the new values of the grid points on both sides of the interface. This value is interpolated from the results of the exact Riemann solver with results from the TVD solver at time step n+1 using the following equations,

$$U_i^{n+1} = \frac{x_i - x_{i-1}}{x_{mi} - x_{i-1}} \left(U_l^* - U_{i-1}^{n+1} \right) + U_{i-1}^{n+1}, \tag{7}$$

$$U_{i+1}^{n+1} = \frac{x_{i+1} - x_{i+2}}{x_{mi} - x_{i+2}} \left(U_r^* - U_{i+2}^{n+1} \right) + U_{i+2}^{n+1}, \tag{8}$$

where values marked with a star are obtained from the exact Riemann solver and include either left or right propagating waves. Equations (7) and (8) are similar to those of Cocchi, et al. [2] except that here the interface location is determined by using the level set functions.

The other correction step is used when the interface propagates to a new location. For example, at time step n+1 it is located between grid points i+1 and i+2 or i and i-1 using Eq. (3) with the level set function calculated for time step n+1. The corrector step as given by Cocchi, et al. [2] for the case when the interface propagates forward is:

$$U_{i+1}^{n+1} = U_l^* . \tag{9}$$

However, here the other grid point must be corrected as well otherwise it will remain diffused. This correction is not included in the procedure employed by Cocchi, et al. [2]. To demonstrate the importance of this correction step a liquid/gas interface propagating at a constant velocity will be discussed. At the time step n+1 the interface location has moved to a new location between grid points i+1 and i+2. The correction step is applied and the liquid parameters at grid point i+1 are obtained. However, the liquid at grid point i is slightly diffused due to the previous interface location, it has lower density and energy than it had previously, at time step n. Therefore, one must correct the results at grid point i as well as those at grid point i+1 otherwise numerical errors are created. The following correction for grid point i is used:

$$U_i^{n+1} = \frac{1}{2} \left(U_l^* + U_{i-1}^{n+1} \right). \tag{10}$$

In addition the parameters γ and B of the equation of state are updated according to the position of the interface according to the values of the level set function at time step n+1. This is performed using Eq. (1).

5 Extension to multidimensional flows

Extension for multi dimensional problems can be done by using an operator splitting technique. This type of extension has been successfully employed by [2, 7] for solving two-dimensional flow fields. Employing this method for two-dimensional flow fields one solves a series of one dimensional problems while retaining the previously described interface correction scheme which is performed after each directional sweep.

$$L_x : U_t + F(U)_x = 0$$
$$L_y : U_t + G(U)_y = 0 \qquad (11)$$
$$U_{i,j}^{n+2} = L_x L_y L_y L_x U_{i,j}^{n}$$

This is in contrast to the method employed by Cocchi and Saurel [3] who solved an exact Riemann problem that was normal to the interface. These results were then interpolated to the Eulerian grid. Using that type of technique is much more complicated and computer intensive. It requires a lot of interpolation, finding the values normal to the interface and using them to compute the exact Riemann problem at the interface. Later these values should be updated based on the results of the exact Riemann problem. In their scheme they employed a front tracking scheme to track the interface. This type of scheme requires many markers to track the interface correctly which further complicates the whole correction procedure. The method proposed here is simpler to use and requires less computation although the correction step should be modified slightly to handle the multi-dimensional interfaces.

6 Numerical Examples

6.1 Shock wave interaction with an oblique gas discontinuity

In this example a planar shock wave of Mach number 2 impinges upon an oblique gaseous wedge with a inclination angle of 50°. This example is taken from Jenny, et al. [4]. The initial conditions and the exact solution near to the location where the incident shock wave interacts with the gaseous wedge are sketched in Figs. 2 and 3, respectively as given by Jenny, et al. [4]. In these figures the dashed line represent the interface between the gases whereas the solid lines represent shock fronts. The numerical simulation was carried out on a uniform grid of 100 x 100 points. The wedge contains high density gas whose density is 5.18 [kg/m^3] and γ=1.1. After some time steps the waves near the interface are shown in Fig. 4. The angles between these waves are similar to the exact solution given by Jenny, et al. [4]. It can be seen that the interface has bent due to the interaction with the shock wave. A transmitted wave is propagating into the heavy gas while a reflected wave is propagating in the opposite direction. The velocity distribution in the x direction is shown in Fig. 5. Smooth velocity profiles appear across the discontinuities in the flow field. This behavior suggests that at the contact discontinuities the flow properties do not generates any oscillations in the flow field.

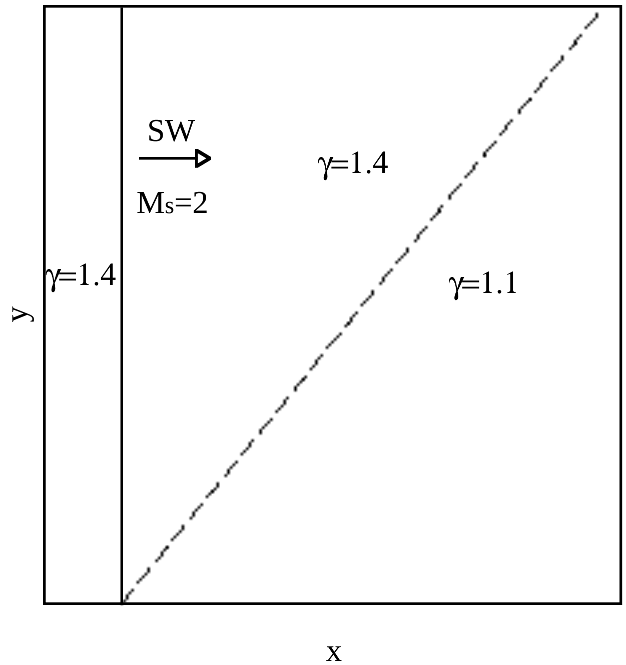

Fig. 2 Initial conditions for shock wave interaction with a gaseous wedge.

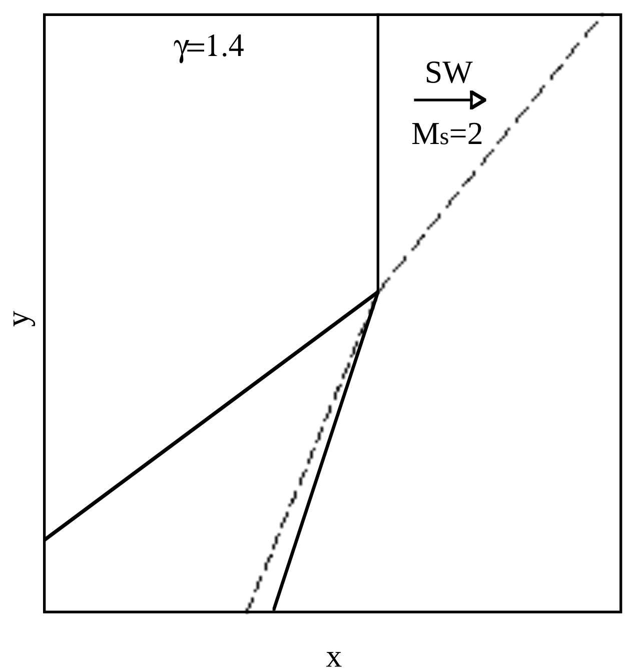

Fig. 3 Final condition of shock wave interaction with a gaseous wedge.

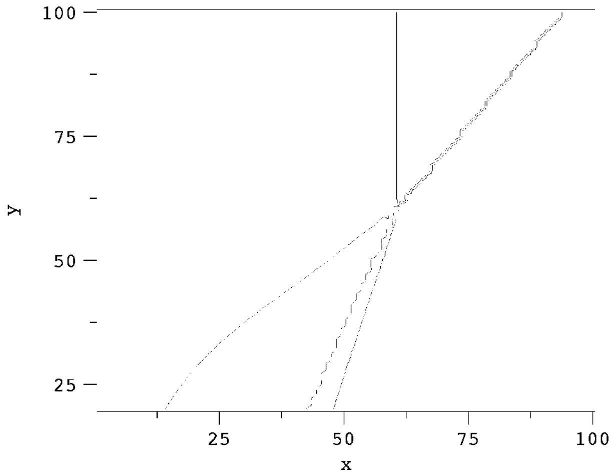

Fig. 4 Location of the main waves.

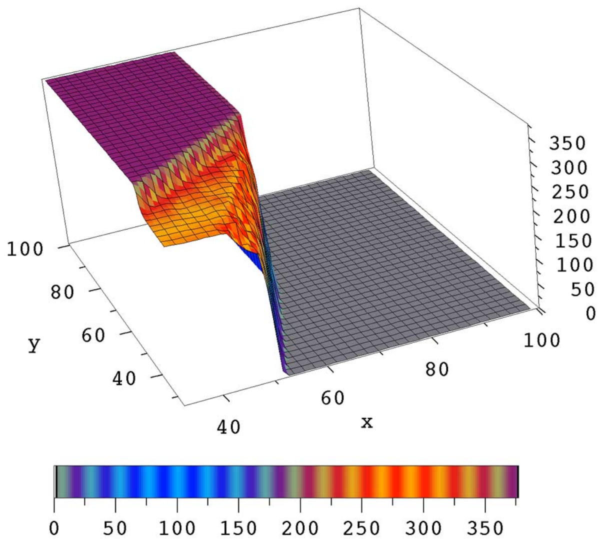

Fig. 5 Velocity distribution in x direction.

6.2 Shock wave interaction with a cylindrical water column

A numerical simulation of a planar shock wave of Mach number 1.3 in air interacting with a cylindrical water column with an initial diameter of 6.4 mm is studied. A schematic diagram of the initial conditions of the flow field is shown in Fig. 6. The CFL number is 0.9 and a minmod limiter was used for all flow fields. A uniform grid of 600 x 300 points with 128 grid points along the water column's radius was used in this simulation. The initial stages of the planar shock wave water column shall be investigated. At these early times the interaction resembles that of a planar shock wave interaction with a solid cylinder. The isopycnics at about 2.5 μs after the incident shock wave impingement on the water column are shown in Fig. 7. The incident shock wave impinged the water column and a regular reflection appears. It is clear that inside the water column a transmitted wave exist, which is a precursory compression wave propagating faster than the shock in air. Due to the higher speed of sound of the water. The difference between the acoustic impedance of the air/water interface results in a small fraction of the energy being transmitted into the water.

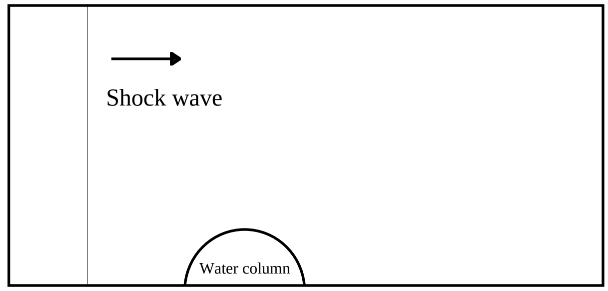

Fig. 6 Schematic diagram of initial conditions of the numerical simulation.

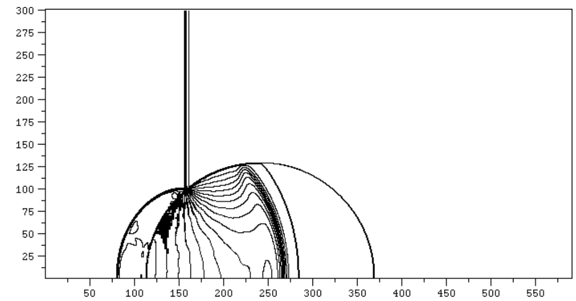

Fig. 7 Isopycnics at t=2.5 μs.

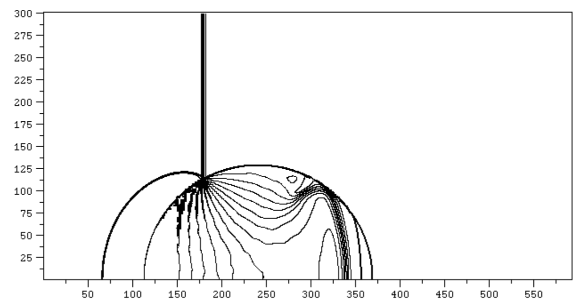

Fig. 8 Isopycnics at t=4.5 μs.

The isopycnics at about 4.5 μs after the incident shock wave impingement on the water column is shown in Fig. 8. The pattern of the reflected wave in air at this point is near its transition from regular to Mach reflection. The precursory wave inside the water column has already propagated more than half way in the water column. A regular reflection appears over the water column. Figure 9 shows the corresponding experimental results, unreconstructed hologram in the bottom; interferogram in the top. Shock waves and gas/liquid interface are clearly seen on the unreconstructed hologram as well as on the interfeogram. Two fringes are observable inside the water column. The shock wave location appear similar to the isopycnics of Fig. 8. The first one is near the frontal part of the water column while the second one is nearly in the middle and is concave towards the direction of propagation. This trend is different from that in Fig. 8.

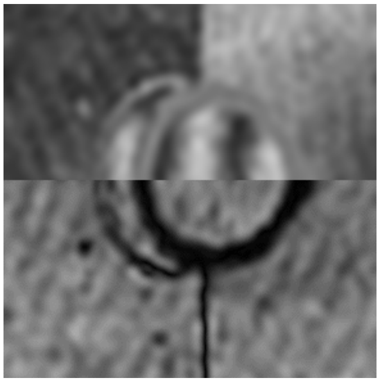

Fig. 9 Experimental results at t=4 μs: interferogram (top); unreconstructed hologram (bottom)

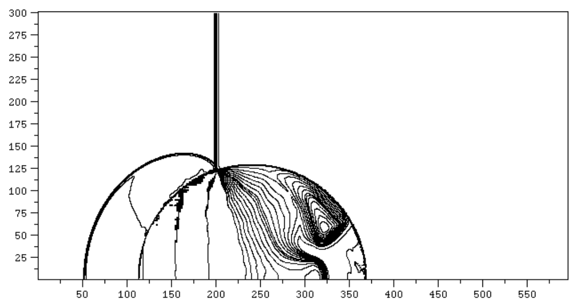

Fig. 10 Isopycnics at t=6 μs.

The isopycnics at about 6 μs is shown in Fig. 10. The precursory transmitted wave is reflected from the air/water interface and reflected expansion wave appears, which converges towards the center. In Fig. 8 the precursory transmitted compression wave is reflected from the interface. The reflected wave is also an expansion wave. The reflection of this wave, after its interaction with boundary compression wave, forms a complex wave system. Along the gas liquid interface the Mach stem is seen. The wave propagation in the water column is similar to that of shock wave focusing in a circular reflector shown by Sun and Takayama [10]. With the elapse of time the waves inside the water column continue to interact with each other leading to complex wave structures. At this early time as shown here the water column retains its cylindrical shape and the flow around it is similar to that of a shock wave interaction with a solid cylinder.

7. Conclusions

The proposed scheme presented here is found to be suitable for handling gas liquid interfaces. It does not create pressure oscillation or density diffusion at the interface. The interface was captured using the level set approach which was added to a system of conservation laws. The numerical scheme was successfully extended for simulating multi dimensional flow fields. In the case of shock wave interaction with a gaseous wedge the location of the waves and contact surfaces agreed well with the exact solution. This scheme was employed to study the shock wave interaction with a water column. The propagation of the transmitted wave inside the water column was investigated. It was found that within a short time a complex wave pattern is generated inside the water column.

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