Numerical Simulation of Compressible Two-Phase Flow Model Based on the Riemann Problem

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Abstract

This paper describes a new approach to the numerical simulation of a one-dimensional isentropic mixture of liquid and vapour without phase change. It amounts to two conservation laws for the mixture coupled by a relative velocity conservation equation. Under certain restrictions the resulting system of conservation law is hyperbolic and allows discontinuous solution. We present high-resolution TVD schemes with an approximate Riemann solver for the resolution of conservation equations. To illustrate the capabilities of the proposed methods, results are presented for carefully chosen test problems. The results show that our numerical schemes are more accurate than other schemes currently used.

Compressible Two-Phase Flow, Riemann Problem, Godunov-type methods

1 Introduction

Computations of complex two-phase flows are required in many industrial areas including safety of nuclear reactors. These computations continue to cause problems for the development of best-estimate computer codes dedicated to improved studies of two-phase flows. To model such flows, several sets of equations ranging in complexity from the homogeneous equilibrium model to two-fluid models involving unequal pressure for each phase have been worked out [1, 3]. The usual way to establish physical modellings for two-phase flows is to start with a single continuous description for each phase given by Navier-Stockes equations. To get computable models, some averaging techniques are used [2]. Generally, this results in ill-posed initial value problems and some differential terms such as virtual mass and interfacial pressure are proposed to make the model hyperbolic [4]. The difficulties associated with the two-fluid model are greatly reduced by using diffusion or homogeneous models, in which the velocity of the two-phase mixture is given by the mixture momentum equation and the relative velocity between phases is expressed by a constitutive equation. This work is concerned with an isentropic mixture twophase flow model, similar to those produced in pressurized water reactor cores. This is a first step to study a more complete model. The purpose of this paper is to solve the Riemann problem for the system and to find an efficient and robust numerical schemes based on the Riemann problem. We present and demonstrate Godunov-type methods of upwind and centred type for solving the isentropic mixture two-fluid model. These methods are conservative shockcapturing TVD (Total-Variation-Diminishing) methods. Moreover, we present two upwind TVD

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schemes, namely the WAF (Weighted Average Flux) scheme and the MUSCL-Hancock (Monotone Upstream-Centred Scheme for Conservation Laws) Method respectively. We then describe a centred TVD scheme, namely the SLIC (Slope LImiter Centre) scheme. As shown in section 3 of this paper, these methods are suitable for various problems such as that of the two-phase shock tube. Further details and other Godunov-type methods can be obtained from [5] and [6].

2 A Simplified Two-Fluid Model of Two-Phase Flow

The isentropic equal pressure two-fluid model consisting in mass and momentum balance equations for each phase take the following form [4]

$$\partial_t(\alpha_j \rho_j) + \partial_x(\alpha_j \rho_j u_j) = 0, \tag{2.1}$$

$$\partial_t(\alpha_i \rho_i u_i) + \partial_x(\alpha_i \rho_i u_i^2) + \alpha_i \partial_x \mathcal{P} = 0. \tag{2.2}$$

In system (2.1) - (2.2), t is the time; x the flow direction; \mathcal{P} is the pressure and ρ_j , u_j and α_j are, respectively, the density, the velocity and the volume fraction of the j-phase (j = 1, 2). We assume no viscosity effect and no mass transfer between phases. In addition, several physical closure laws must be given which involve mass vapour concentration, equation of state for the two-phase flow, mixture relations and properties of the model. Due to space limitation we do not state these models here, but refer instead to [6] for details. More precisely, the system considered in this study can be written as a system of conservation laws as

$$\partial_{\mathbf{t}} \mathbb{U} + \partial_{\mathbf{x}} \mathbb{F}(\mathbb{U}) = \mathbf{0}, \tag{2.3}$$

with

$$\mathbb{U} = \begin{pmatrix} \rho \\ \rho u \\ u_r \end{pmatrix}, \tag{2.4}$$

and the flux function

$$\mathbb{F}(\mathbb{U}) = \begin{pmatrix} \rho u \\ \rho u^2 + \rho \ c \ (1 - c) \ u_r^2 + \mathcal{P} \\ u u_r + \frac{1 - 2c}{2} \ u_r^2 + \psi(\mathcal{P}) \end{pmatrix}, \tag{2.5}$$

where u_r is the relative velocity between the two phases. This conservative form of the simplified one-dimensional model, although derived for a smooth solution \mathbb{U} , will be useful to define jump conditions for the approximate Riemann solver to build more efficient Godunov-type numerical methods.

Equation (2.3) can be linearized in terms of primitive-variable formulations. Primitive formulations of the mixture two-fluid model have a much simpler form than the conservative formulations. Also, from a numerical point of view, numerical schemes based on a primitive formulation are more efficient. One possible primitive formulation of the simplified two-fluid model is the following

$$\partial_t \mathbb{W} + \mathbb{A}(\mathbb{W})\partial_x \mathbb{W} = 0, \tag{2.6}$$

where the primitive state vector \mathbb{W} is taken as $\mathbb{W} = (\mathcal{P}, u, u_r)^T$. Mathematical properties of system (2.3) - (2.5) were studied by Zeidan [6]. The model was shown to be hyperbolic (using

perturbation methods) in a physically reasonable region of parameters and three distinct and real eigenvalues were obtained under the assumption that the relative velocity between the two phases is much lower than the speed of sound, a_m , of the two-phase mixture (i.e. $\eta = \frac{u_r}{a_m} \ll 1$) which is the case in many physically interesting mixtures such as steam and water.

3 Riemann-Problem-Based Shock Capturing Schemes

For numerical solution of this initial-boundary value problem (Eq. (2.3)) with the initial conditions $\mathbb{U}(x,0) = \mathbb{U}^{(0)}(x)$ and the general boundary conditions $L(t)\mathbb{U}(0,t) = f(t)$, $R(t)\mathbb{U}(L,t) = g(t)$ where L, R are given matrices and f(t), g(t) are given functions, we use a conservative finite volume method for which the (x,t)-space is descretized uniformly in cells of size Δx and Δt . The discrete point x_i denote the cell centres and the point $x_{i+\frac{1}{2}}$ the cell boundaries. All the schemes are based on the explicit conservative formula to solve Eq. (2.3), namely

$$\mathbb{U}_{i}^{n+1} = \mathbb{U}_{i}^{n} - \frac{\Delta t}{\Delta x} \left[\mathbb{F}_{i+\frac{1}{2}} - \mathbb{F}_{i-\frac{1}{2}} \right]. \tag{3.7}$$

 $\mathbb{F}_{\mathfrak{i}+\frac{1}{2}}$ is the inter-cell flux corresponding to the inter-cell boundary at $x=x_{\mathfrak{i}+\frac{1}{2}}$ between cells \mathfrak{i} and $\mathfrak{i}+1$. The choice of the time step Δt in Eq. (3.7) satisfies the condition

$$\Delta t = C \frac{\Delta x}{\mathbb{S}_{max}^{(n)}},\tag{3.8}$$

where C is the CFL (Courant-Friedrichs-Lewy) number with $0 < C \le 1$ and $\mathbb{S}_{max}^{(n)}$ is the maximum wave speed present at time level n chosen as [6]

$$\mathbb{S}_{max}^{(n)} = \max_{i} \left\{ |u_{i}^{n}| + a_{mi}^{n} + \frac{\rho_{i}^{n}}{\rho_{21i}^{n}} c_{i}^{n} (1 - c_{i}^{n}) u_{ri}^{n} \right\}.$$
(3.9)

The choice of the numerical flux $\mathbb{F}_{i+\frac{1}{2}}$ determines the scheme which follows the basic ideas of Toro [5] for the resolution of Euler equations. In the following we extended these schemes to compressible two-phase flow calculations. We present a new numerical method for two-phase flow computations that is based on an approximate Riemann solver. It uses the solution of a one-dimensional Riemann problem at cell interfaces to define Godunov-type numerical schemes. The basic idea is to update the conserved variables according to the conservative formula of Eq. (3.7). Further, we briefly describe our approximate Riemann solver, the HLLC (Harten, Lax van Leer and Contact), for the simplified two-fluid model. Then we describe two upwind-based second order TVD schemes based on the approximate solver, and demonstrate a TVD centred (non-upwind) scheme for the simplified two-fluid model. Further details on the numerical solutions can be found in [6].

3.1 HLLC-Type Approximations Riemann Solver

To solve the nonlinear Riemann problem Eq. (2.3) for hyperbolic systems of conservation laws, we construct a HLLC Riemann solver to solve the simplified two-fluid model. Our HLLC Riemann solver is accurate and robust in comparison with other approximate Riemann solvers such as Roe's solver which would require an explicit entropy fix. In addition, the HLLC Riemann solver forms the basis of very efficient and robust approximate Godunov-type methods. The HLLC Riemann solver assumes an estimate of the left and right wave speed \mathbb{S}^- and \mathbb{S}^+ at cell boundary and an estimate \mathbb{S}^* for the speed of the middle wave which is $\mathbb{S}^* = \lambda_2$ up to first order in η in

the exact Riemann solver [6]. Assuming all wave speed estimates are available we can derive the HLLC numerical flux as

$$\mathbb{F}_{i+\frac{1}{2}}^{hllc} = \begin{cases}
\mathbb{F}_{\mathcal{L}}, & \text{if } 0 \leq \mathbb{S}_{\mathcal{L}}, \\
\mathbb{F}_{\mathcal{L}}^{\star}, & \text{if } \mathbb{S}_{\mathcal{L}} \leq 0 \leq \mathbb{S}^{\star}, \\
\mathbb{F}_{\mathcal{R}}^{\star}, & \text{if } \mathbb{S}^{\star} \leq 0 \leq \mathbb{S}_{\mathcal{R}}, \\
\mathbb{F}_{\mathcal{R}}, & \text{if } 0 \geq \mathbb{S}^{\mathcal{R}},
\end{cases}$$
(3.10)

where

$$\mathbb{F}_{\mathcal{L}}^{\star} = \mathbb{F}_{\mathcal{L}} + \mathbb{S}_{\mathcal{L}}(\mathbb{U}_{\mathcal{L}}^{\star} - \mathbb{U}_{\mathcal{L}}), \tag{3.11}$$

$$\mathbb{F}_{\mathcal{L}}^{\star} = \mathbb{F}_{\mathcal{L}} + \mathbb{S}_{\mathcal{L}}(\mathbb{U}_{\mathcal{L}}^{\star} - \mathbb{U}_{\mathcal{L}}),
\mathbb{F}_{\mathcal{R}}^{\star} = \mathbb{F}_{\mathcal{R}} + \mathbb{S}_{\mathcal{R}}(\mathbb{U}_{\mathcal{R}}^{\star} - \mathbb{U}_{\mathcal{R}}).$$
(3.11)

The states $\mathbb{U}_{\mathcal{L}}^{\star}$ and $\mathbb{U}_{\mathcal{R}}^{\star}$ are given by

$$\mathbb{U}_{k}^{\star} = \rho_{k} \left(\frac{\mathbb{S}_{k} - u_{k}}{\mathbb{S}_{k} - \mathbb{S}^{\star}} \right) \left(\frac{\mathbb{S}_{k} - u_{k}}{\mathbb{S}_{k} - \mathbb{S}^{\star}} \frac{u_{rk}}{\rho_{k}^{\star}} + \frac{1}{\rho_{k}^{\star}(\mathbb{S}_{k} - \mathbb{S}^{\star})} \left[\frac{1 - 2c^{\star}}{2} u_{rk}^{2\star} - \frac{1 - 2c_{k}}{2} u_{rk}^{2} + \psi(\mathbb{P}_{k}^{\star}) - \psi(\mathbb{P}_{k}) \right] \right), \tag{3.13}$$

obtained from manipulating relations (3.11) and (3.12) with $k = \mathcal{L}, \mathcal{R}$.

Shock-Capturing Upwind Methods 3.2

Here we describe a second-order accuracy for the numerical fluxes using high-resolution TVD upwind schemes namely the WAF and the MUSCL-Hancock scheme respectively.

3.2.1 The Weighted Average Flux (WAF) Scheme

The WAF method is a second-order extension of the Godunov-upwind method. The basic idea behind WAF method was first developed for the Euler equations [5]. Here we consider a TVD version of WAF method. The resulting TVD WAF flux is

$$\mathbb{F}_{i+\frac{1}{2}} = \frac{1}{2} (\mathbb{F}_{i} + \mathbb{F}_{i+1}) - \frac{1}{2} \sum_{k=1}^{N} sign(C_k) \phi_{i+\frac{1}{2}}^{(k)} \Delta \mathbb{F}_{i+\frac{1}{2}}^{(k)}, \tag{3.14}$$

where $\phi_{i+\frac{1}{2}}^{(k)} = \phi_{i+\frac{1}{2}}(r^{(k)})$ is a WAF limiter function which is designed to ensure the method is TVD. The parameter $r^{(k)}$ refers to wave k in the solution $\mathbb{U}_{\mathfrak{i}+\frac{1}{2}}(x,t)$ of the Riemann problem and is the ratio

$$r^{(k)} = \begin{cases} \frac{\Delta q_{i-\frac{1}{2}}^{(k)}}{\Delta q_{i+\frac{1}{2}}^{(k)}}, & \text{if } C_{(k)} > 0, \\ \frac{\Delta q_{i+\frac{3}{2}}^{(k)}}{\Delta q_{i+\frac{1}{2}}^{(k)}}, & \text{if } C_{(k)} < 0, \end{cases}$$

$$(3.15)$$

where q is known to change across each wave family in the solution of the Riemann problem. For the simplified two-fluid model $q = u_r$ give very sufficient results. There exists a variety

of limiters that can be used to calculate the slops in the WAF method. We refer to [5] for a detailed description of the available limiters. In this paper we will only use SUPERBEE limiter which is known to be overcompressive (i.e. tends to sharpen profiles into discontinuities). The SUPERBEE limiter given by

$$\phi(r,|C|) = \begin{cases} 1 & \text{if} & r \leq 0, \\ 1 - 2(1 - |C|)r & \text{if} & 0 \leq r \leq \frac{1}{2}, \\ |C| & \text{if} & \frac{1}{2} \leq r \leq 1, \\ 1 - (1 - |C|)r & \text{if} & 1 \leq r \leq 2, \\ 2|C| - 1 & \text{if} & r \geq 2, \end{cases}$$
(3.16)

is equivalent to a conventional flux limiter $\psi(r)$ since $\phi(r) = (1 - (1 - |C|))\psi(r)$ where $\psi(r) = max((0, min(2r, 1), min(r, 2))$.

3.2.2 The MUSCL-Hancock Method

The MUSCL-Hancock scheme is another second-order extension of the Godunov upwind scheme. The basis of MUSCL-Hancock scheme is the reconstruction of piecewise constant data \mathbb{W}_i^n into a piecewise linear distribution of the data (i.e. $\mathbb{W}_i(x) = \mathbb{W}_i^n + (x - x_i) \frac{\Delta_i}{\Delta x}$, $x \in I_i$, where $x_i = (i - \frac{1}{2})\Delta x$ is the centre of the computing cells I_i , Δ_i are the slopes of three components for the simplified two-fluid model) and then to extrapolate the data to the edges of each cell, yielding the extrapolated values $\mathbb{W}_i^{\mathcal{L}}$, $\mathbb{W}_i^{\mathcal{R}}$. The extrapolated values are then evolved through a half time step according to the primitive formulae $\overline{\mathbb{W}}_i^{\mathcal{L},\mathcal{R}} = \mathbb{W}_i^{\mathcal{L},\mathcal{R}} - \frac{1}{2} \frac{\Delta t}{\Delta x} \mathbb{A}_i^n [\mathbb{W}_i^{\mathcal{R}} - \mathbb{W}_i^{\mathcal{L}}]$, where \mathbb{A}_i^n denotes the matrix $\mathbb{A}(\mathbb{W})$ in Eq. (2.6). In the third step, we solve a conventional piecewise constant data Riemann problem with initial data consisting of evolved boundary extrapolated values, i.e., the inter-cell flux \mathbb{F}_i is now computed as $\mathbb{F}_i = \mathbb{F}(\mathbb{W}_{i+\frac{1}{2}}(0))$. Finally, to avoid the expected spurious oscillations, a TVD constraint is enforced in the data reconstruction step by limiting the slopes Δ_i by $\overline{\Delta}_i$. We refer to [5, 6] for further approaches on the slopes $\overline{\Delta}_i$. The SUPERBEE limiter was used in the paper.

3.3 Shock-Capturing Centred Schemes

Centred methods are methods that do not require the explicite solution of the Riemann problem, i.e., they are not biased by the wave propagation direction. We present here a second-order TVD scheme that is an extension of the FORCE (First-Order Centred) scheme. The scheme is of the slop limiter type (The Slope LImiter Centred, SLIC, scheme) and results from replacing the Godunov flux by the FORCE flux in the MUSCL-Hancock scheme [5, 6]. The SLIC scheme is realized by three steps. Step (I) and (II) are exactly the same as in the MUSCL-Hancock scheme. The first step results in boundary extrapolated values

$$\mathbb{U}_{i}^{\mathcal{L}} = \mathbb{U}_{i}^{n} - \frac{1}{2}\Delta_{i}; \ \mathbb{U}_{i}^{\mathcal{R}} = \mathbb{U}_{i}^{n} + \frac{1}{2}\Delta_{i}, \tag{3.17}$$

in each cell I_i , where Δ_i is a vector difference of neighbouring states given by the average between inter-cells slopes

$$\mathbb{W}_{i-\frac{1}{2}} = \mathbb{W}_{i}^{n} - \mathbb{W}_{i-1}^{n}, \ \mathbb{W}_{i+\frac{1}{2}} = \mathbb{W}_{i+1}^{n} - \mathbb{W}_{i}^{n}, \tag{3.18}$$

namely

$$\Delta_{i} = \frac{1}{2}(1+\omega)\Delta_{i-\frac{1}{2}} + \frac{1}{2}(1-\omega)\Delta_{i+\frac{1}{2}},$$
(3.19)

where the parameter $\omega \in [-1,1]$ for the simplified two-fluid model $\omega = 0$. $\Delta_{\mathfrak{i}-\frac{1}{2}}$, $\Delta_{\mathfrak{i}+\frac{1}{2}}$ denote jumps across interfaces $\mathfrak{i}-\frac{1}{2}$ and $\mathfrak{i}+\frac{1}{2}$ given by

$$\Delta_{\mathfrak{i}-\frac{1}{2}} \equiv \mathbb{U}_{\mathfrak{i}}^{n} - \mathbb{U}_{\mathfrak{i}-1}^{n}; \ \Delta_{\mathfrak{i}+\frac{1}{2}} \equiv \mathbb{U}_{\mathfrak{i}+1}^{n} - \mathbb{U}_{\mathfrak{i}}^{n}. \tag{3.20}$$

The second step evolves $\mathbb{U}_i^{\mathcal{L}}$, $\mathbb{U}_i^{\mathcal{R}}$ by a half time step according to

$$\overline{\mathbb{U}}_{i}^{\mathcal{L}} = \mathbb{U}_{i}^{\mathcal{L}} + \frac{1}{2} \frac{\Delta t}{\Delta x} [\mathbb{F}(\mathbb{U}_{i}^{\mathcal{L}}) - \mathbb{F}(\mathbb{U}_{i}^{\mathcal{R}})], \tag{3.21}$$

$$\overline{\mathbb{U}}_{i}^{\mathcal{R}} = \mathbb{U}_{i}^{\mathcal{R}} + \frac{1}{2} \frac{\Delta t}{\Delta x} [\mathbb{F}(\mathbb{U}_{i}^{\mathcal{L}}) - \mathbb{F}(\mathbb{U}_{i}^{\mathcal{R}})]. \tag{3.22}$$

In step(III), instead of solving the Riemann problem with data $\mathbb{W}_{\mathcal{L}} \equiv \overline{\mathbb{U}}_{i}^{\mathcal{R}}$; $\mathbb{W}_{\mathcal{R}} \equiv \overline{\mathbb{U}}_{i}^{\mathcal{L}}$ to find the Godunov flux at the inter-cell position $\mathfrak{i} + \frac{1}{2}$, we evaluate the FORCE flux

$$\mathbb{F}_{i+\frac{1}{2}}^{force} = \mathbb{F}_{i+\frac{1}{2}}^{force}(\overline{\mathbb{U}}_{i}^{\mathcal{R}}, \overline{\mathbb{U}}_{i+1}^{\mathcal{L}}), \tag{3.23}$$

where FORCE flux given by

$$\mathbb{F}_{i+\frac{1}{2}}^{force} = \mathbb{F}_{i+\frac{1}{2}}^{force}(\mathbb{U}_{\mathcal{L}}, \mathbb{U}_{\mathcal{R}}) = \frac{1}{2} [\mathbb{F}_{i+\frac{1}{2}}^{LF}(\mathbb{U}_{\mathcal{L}}, \mathbb{U}_{\mathcal{R}}) + \mathbb{F}_{i+\frac{1}{2}}^{RI}(\mathbb{U}_{\mathcal{L}}, \mathbb{U}_{\mathcal{R}})]. \tag{3.24}$$

In implementing the TVD version of the scheme for the simplified two-fluid model the slopes Δ_i are replaced by slops $\overline{\Delta_i}$ with the SUPERBEE limiter.

4 Numerical Results

We present two sets of numerical results obtained with TVD centred schemes and high-resolution upwind based on HLLC Riemann solver. A precise description of the parameters involved is given in [6]. We have chosen to present plots of the WAF scheme as a shock-capturing upwind method and a SLIC method as a shock-capturing centred scheme. The MUSCL-Hancock method were successfully applied and plotted in [6]. The test problems were applied to a two-fluid shock-tube problem [6], consisting of a Riemann problem with transmissive boundary conditions in which there are three wave families as a part of the solution. The first test problem is characetrized by a left sonic rarefaction and a right shock wave. Feature of this test is that the left rarefaction is sonic (or critical), i.e., the eigenvalue $\lambda_1 = u - a_m + \frac{\rho}{\rho_{21}}c(1-c)u_r + a_m\mathfrak{O}(\eta^2)$ changes from negative value to a positive value as the wave is crossed from left to right, see Figs. 1, 2 and 3. The second test deals with a solution consisting of a single left shock wave associated with the left eigenvalue and a right rarefaction wave associated with the right eigenvalue separated by a contact discontinuity, see Figs. 4, 5 and 6. Figs. 1 and 4 of Test 1 and Test 2 correspond to the WAF method of Sect. 3.2 with the HLLC approximate Riemann solver of Sect. 3.1 using the flux limiter function SUPERBEE (3.16). The results gives a very sharp resolution of discontinuities but small spurious oscillations are just visible on the plots. Fig. 2 of Test 1 and Fig. 5 of Test 2 show results from the SLIC scheme with the SUPERBEE limiter. The results are less accurate than those from the WAF scheme. As expected, the Lax-Friedrichs scheme (see Figs. 3 and 6 of Test 1 and 2) has much more numerical diffusion than the other numerical schemes, but the results obtained with the two schemes are in good agreement.

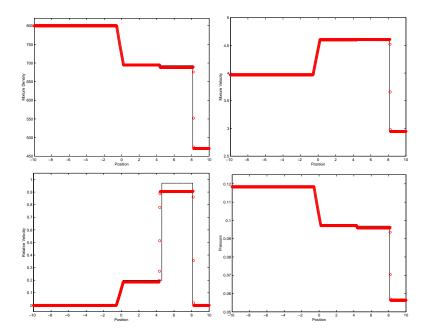


Figure 1: WAF scheme with HLLC Riemann solver and SUPERBEE TVD function applied to Test 1. Numerical (symbol) and exact (line) solutions are compared at t=1.0.

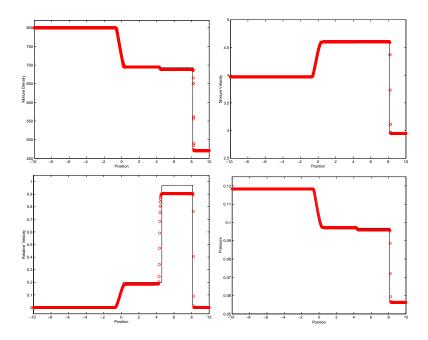


Figure 2: Slope LImiter Centred (SLIC) scheme with SUPERBEE TVD function applied to Test 1. Numerical (symbol) and exact (line) solutions are compared at t=1.0.

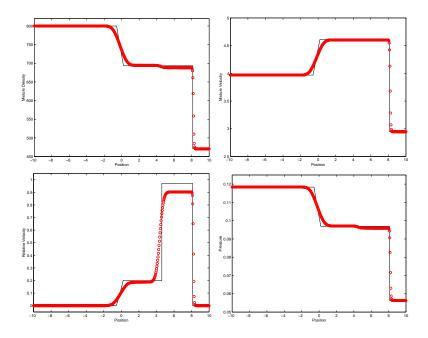


Figure 3: Lax-Friedrichs scheme applied to Test 1. Numerical (symbol) and exact (line) solutions are compared at t = 1.0.

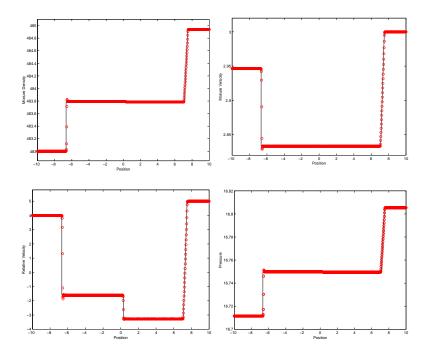


Figure 4: WAF scheme with HLLC Riemann solver and SUPERBEE TVD function applied to Test 2. Numerical (symbol) and exact (line) solutions are compared at t = 0.1.

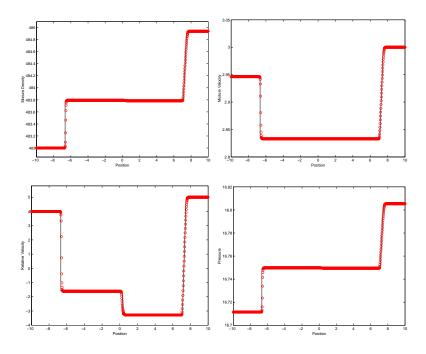


Figure 5: Slope LImiter Centred (SLIC) scheme with SUPERBEE TVD function applied to Test 2. Numerical (symbol) and exact (line) solutions are compared at t=0.1.

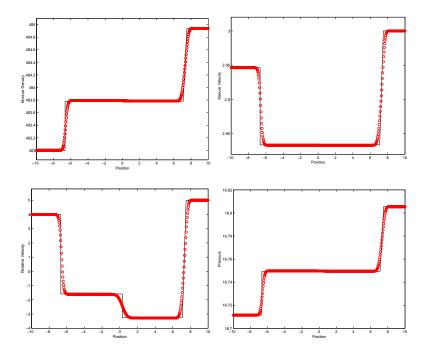


Figure 6: Lax-Friedrichs scheme applied to Test 2. Numerical (symbol) and exact (line) solutions are compared at t=0.1.

5 Conclusion

An extension of the Godunov-type methods have been developed. It allows the numerical resolution of compressible two-phase flow with constitutive equation. It is a second order conservative TVD schemes combined with an approximate Riemann solver. The efficiency of the subsequent methods have been demonstrated on difficult test problems. The methods are accurate, robust and they are expected to provide an efficient way to calculate more realistic two-phase flow problems.

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