The Role of Coordinates in the Computation of Discontinuities in One-Dimensional Flow

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Abstract

Two coordinate systems have been widely used to describe fluid flow: the Eulerian and the Lagrangian. Analytically, both systems are capable of producing exact solutions including discontinuities, and they are largely equivalent to each other, except that the Lagrangian system gives more information: the history of each fluid particle. Computationally, however, the two systems behave quite differently, especially for flows with discontinuities. Eulerian computation tends to smear slip lines (or contact lines) badly, whereas Lagrangian computation may break down due to severe deformation of computational cells which are identical to fluid particles.

A unified coordinate system is introduced where the computational cells move with velocity hu, u being the fluid velocity. It is used to study the role of coordinates in resolving one-dimensional flow discontinuities, i.e. shocks and slip lines, by varying the value of h from $h = 0$ (Eulerian) to $h = 1$ (Lagrangian).

Systematic study using Godunov-type shock capturing schemes on six 1-D test problems and a piston problem shows that **(a)** slip line resolution is very poor for Eulerian coordinates ($h = 0$) but improves with increasing h, reaching the optimum when $h = 1$ (Lagrangian coordinates), **(b)** numerical smearing of shocks is independent of h but, **(c)** with the Lagrangian coordinates, a shock-adaptive Godunov scheme can be applied to yield infinite shock resolution. Consequently, Lagrangian coordinate system with a shock-adaptive Godunov scheme produces the best result for the one-dimensional Euler equations of gas dynamics.

1 Introduction

There exist two different coordinate systems for description of fluid motion: the Eulerian one describes fluid motion at fixed locations, whereas the Lagrangian one does so following fluid particles. Accordingly, the Eulerian description considers velocities and other properties of fluid particles to be functions of time and of fixed space coordinates. In contrast, the Lagrangian description considers the positions of fluid particles and their other properties to be functions of time and of their permanent identifications, such as their initial positions or any set of material functions of fluid particles. Both coordinate systems are capable of producing exact analytical solutions of fluid flows, including discontinuous flows. They are regarded as equivalent to each other (for one-dimensional flow, the equivalency was proved rigorously by Wagner [1]), except that the Lagrangian one gives more information: it tells each fluid particle's history. They are not equivalent from numerical computation point of view.

Computationally, in using Eulerian coordinates the computational cells are fixed in space, while fluid particles move across cell interfaces. It is this convective flux that causes excessive numerical diffusion in the numerical solutions with flow discontinuities. Indeed, slip lines (also called contact lines) are smeared badly and shocks are also smeared, albeit somewhat better than slip lines. Moreover, the smearing of slip lines ever increases with time and distance unless special treatments, such as artificial compression or sub-cell resolution, are introduced [2-4] which are, however, not always reliable. The primary efforts of the CFD algorithm researchers since the sixties have concentrated on developing better (more robust, accurate and efficient) ways to deal with this convective flux. Although great progresses have been made and "perhaps to the point of near perfection and little return could be gained" [5], numerical diffusion still exists, causing inaccuracy.

Computational cells in the Lagrangian coordinates, on the other hand, are literally fluid particles. Consequently, there is no convective flux across cell boundaries and the numerical diffusion is thus minimized. However, the very fact that computational cells

behave exactly like fluid particles can result in grid deformation so severe that the computation may break down in multi-dimensional flow. To prevent this from happening, the most famous Lagrangian method in use at present time - the Arbitrary Lagrangian - Eulerian Technique (ALE)[6-8] - uses continuous re-zoning and re-mapping to the Eulerian grid. Unfortunately, this process requires interpolations of geometry and flow variables which result in loss of accuracy, manifested as numerical diffusion which ALE wants to avoid in the first place. Indeed, it was demonstrated in [9] that re-zoning results in diffusive errors of the type encountered in Eulerian solutions and continuously re-zoned Lagrangian computation is equivalent to an Eulerian computation.

After a series of study [10-18] on steady supersonic flow, Hui et.al.[19] have recently introduced a new description of unsteady fluid motion in which the flow variables (velocities, pressure, density, etc.) are considered to be functions of time and of some permanent identifications of **pseudo-particles** which move with velocity $h\mathbf{q}$, $\mathbf{q}$ being velocity of fluid particles. This turns out to be a unified description, ranging from Eulerian when $h = 0$ to Lagrangian when $h = 1$, but the freedom in choosing h makes it possible to avoid the disadvantages of excessive diffusion across slip lines in Eulerian description and, in the case of multi-dimensional flow, of severe grid deformation in Lagrangian description. For two-dimensional flow, h may also be chosen to produce an orthogonal grid, which would be the optimal.

In this paper we shall use the unified coordinates to study the role of coordinate system in the numerical resolution of flow discontinuities in one-dimensional unsteady flow as modeled by the Euler equations of gas dynamics. The counter-part for two-dimensional flow is given in [19].

In section 2, the Euler equations will be written in the unified coordinates. Section 3 explains the solution to the Riemann problem, which will be used in the unified computer code in section 5. Section 4 describes the shock-adaptive Godunov scheme for improving resolution of shocks. Numerical results produced by the unified code are given in section 6 for seven test problems and are compared for different systems of coordinates. Finally,

conclusions are given in section 7.

2 One-Dimensional Euler Equations Written in the Unified Coordinates

As our goal is to investigate the quality of computed solutions obtained in different coordinates, a unified code for arbitrary h will be written to carry out this task. But before describing the code we first discuss the mathematical properties of the system of 1-D unsteady Euler equations written in the unified coordinates.

The 1-D unsteady Euler equations in conservation form written in cartesian coordinates are

$$\frac{\partial \mathbf{E_e}}{\partial t} + \frac{\partial \mathbf{F_e}}{\partial x} = 0 \tag{1}$$

where

$$\mathbf{E_e} = \begin{bmatrix} \rho \\ \rho u \\ \rho e \end{bmatrix}, \quad \mathbf{F_e} = \begin{bmatrix} \rho u \\ \rho u^2 + p \\ \rho u H \end{bmatrix} \tag{2}$$

In (2), ρ is the density, p the pressure, u the velocity, γ the ratio of specific heats of the gas, and

$$e = \frac{u^2}{2} + \frac{p}{(\gamma - 1)\rho}, \quad H = e + \frac{p}{\rho} \tag{3}$$

Consider the following transformation of variables

$$\begin{cases} dt = d\lambda \\ dx = hud\lambda + Ad\xi \end{cases} \tag{4}$$

where $h(\lambda, \xi)$ is an arbitrary function. It can easily be shown that

$$\frac{\partial \xi}{\partial t} + hu\frac{\partial \xi}{\partial x} = 0. \tag{5}$$

This means that the coordinate ξ is invariant following a **pseudo-particle** whose velocity is hu. Consequently, computational cells move with the pseudo-particles, instead of the

fluid particles as in Lagrangian coordinates. As we can see from the above transformation, the case $h = 0$ gives us the Eulerian coordinates in which ξ is independent of the flow; in particular, $\xi = x$ if $A = 1$. On the other hand, the case $h = 1$ gives the Lagrangian coordinates, since the pseudo-particles are identical to the fluid particles. The advantage of this unified coordinate system is its ability to show the effect of coordinate systems on the behaviour of the solution by simply varying the parameter h from 0 to 1.

Under the above transformation, system (1) becomes

$$\frac{\partial \mathbf{E}}{\partial \lambda} + \frac{\partial \mathbf{F}}{\partial \xi} = 0 \tag{6}$$

where

$$\mathbf{E} = \begin{bmatrix} \rho A \\ \rho A u \\ \rho A e \\ A \end{bmatrix}, \quad \mathbf{F} = \begin{bmatrix} (1-h)\rho u \\ (1-h)\rho u^2 + p \\ (1-h)\rho u e + up \\ -hu \end{bmatrix} \tag{7}$$

The last equation in (7) is the compatibility condition of the differential relation (4) for dx.

It is well-known that system (1) is hyperbolic in t-direction. We now prove that system (6) is also hyperbolic in λ-direction, despite the fact that the transformation involves the unknown function u. We choose $\mathbf{Q} = (p, \rho, u, A)^T$ to be the vector of state variables, then for smooth solutions system (6) can be written as

$$\mathbf{A}\frac{\partial \mathbf{Q}}{\partial \lambda} + \mathbf{B}\frac{\partial \mathbf{Q}}{\partial \xi} = \mathbf{R} \tag{8}$$

where $\mathbf{R} = (0, 0, 0, uh_\xi)^T$ and

$$\mathbf{A} = \frac{\partial \mathbf{E}}{\partial \mathbf{Q}} = \begin{pmatrix} 0 & D\lambda & \lambda_x \rho & 0 \\ \lambda_x & uD\lambda & \lambda_x \rho u + \rho D\lambda & 0 \\ \frac{\gamma}{\gamma-1}D\lambda - \lambda_t & \frac{u^2}{2}D\lambda & \rho u D\lambda + \lambda_x \rho H & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \tag{9}$$

$$\mathbf{B} = \frac{\partial \mathbf{F}}{\partial \mathbf{Q}} = \begin{pmatrix} 0 & D\xi & \xi_x \rho & 0 \\ \xi_x & uD\xi & \xi_x \rho u + \rho D\xi & 0 \\ \frac{\gamma}{\gamma-1} D\xi - \xi_t & \frac{u^2}{2} D\xi & \rho u D\xi + \xi_x \rho H & 0 \\ 0 & 0 & -h & 0 \end{pmatrix} \tag{10}$$

where

$$D\lambda = \lambda_t + u\lambda_x \tag{11}$$

$$D\xi = \xi_t + u\xi_x \tag{12}$$

The eigenvalues σ are to be found from the vanishing of $det(\sigma \mathbf{A} - \mathbf{B})$, where

$$(\sigma \mathbf{A} - \mathbf{B}) = \begin{pmatrix} 0 & m & \beta\rho & 0 \\ \beta & um & \beta\rho u + \rho m & 0 \\ \frac{\gamma m}{\gamma-1} - \mu & \frac{u^2}{2} m & \rho u m + \beta \rho H & 0 \\ 0 & 0 & h & \sigma \end{pmatrix} \tag{13}$$

with

$$m = \sigma + (1-h)\beta u \tag{14}$$

$$\mu = \sigma\lambda_t - \xi_t \tag{15}$$

$$\beta = \sigma\lambda_x - \xi_x \tag{16}$$

Direct computation gives

$$det(\sigma \mathbf{A} - \mathbf{B}) = \frac{\sigma \rho m}{\gamma - 1}(m^2 - \beta^2 a^2), \tag{17}$$

hence the eigenvalues are (for $0 \leq h \leq 1$)

$$(i) \quad \sigma = 0 \tag{18}$$

$$(ii) \quad \sigma = \frac{(1-h)u}{A} \tag{19}$$

$$(iii) \quad \sigma_\pm = \frac{(1-h)u \pm a}{A} \tag{20}$$

where $a = (\frac{\gamma p}{\rho})^{1/2}$ is the speed of sound. The corresponding right eigenvectors are

$$\mathbf{r_1} = (0,0,0,1)^T \tag{21}$$

$$\mathbf{r_2} = (0,1,0,0)^T \tag{22}$$

$$\mathbf{r}_\pm = (1, a^{-2}, \pm\frac{1}{a\rho}, \mp\frac{h}{a\rho\sigma_\pm})^T \tag{23}$$

Since these eigenvectors are evidently linearly independent, we conclude that system (6) is **hyperbolic in λ-direction**.

We shall use a Godunov-type scheme to solve the Euler equation (6) for constant, but arbitrary, h: $0 \leq h \leq 1$. This requires the solution to the Riemann problem.

3 Riemann Problem for the Euler Equations written in Unified Coordinates

The Riemann problem for one-dimensional unsteady flow written in the unified coordinates is

$$\begin{cases} \frac{\partial \mathbf{E}}{\partial \lambda} + \frac{\partial \mathbf{F}}{\partial \xi} = 0 & \lambda > 0 \\ \mathbf{Q}(0,\xi) = \begin{cases} \mathbf{Q}_\mathbf{l}, & \xi < 0 \\ \mathbf{Q}_\mathbf{r}, & \xi > 0 \end{cases} \end{cases} \tag{24}$$

where $\mathbf{Q}_\mathbf{l}$ and$\mathbf{Q}_\mathbf{r}$ are the constant vectors representing the flow states on the left and right side, respectively. From now on, we shall consider only the simpler case when h is a constant in the range $0 \leq h \leq 1$. The general case when h is a function of the coordinates is discussed in [19]. With $h = const.$, eq.(24) is a system of conservation law equations with constant coefficients and a solution to the Riemann problem depends on $\zeta = \frac{\lambda}{\xi}$ alone, i.e. it is a self-similar solution of the form $\mathbf{Q} = \mathbf{Q}(\zeta)$. It is constructed by piecing the smooth solutions with the discontinuous solutions.

3.1 Nonlinearity of Characteristic Fields

Case 1 $\sigma_1 = 0$

We have

$$\mathbf{r_1} \cdot \nabla \sigma_1 = 0 \tag{25}$$

Hence, the characteristic field corresponding to $\sigma_1 = 0$ is linearly degenerate.

Case 2 $\sigma_2 = \frac{(1-h)u}{A}$

We have

$$\mathbf{r_2} \cdot \nabla \sigma_2 = (\frac{(1-h)u}{A})_\rho = 0 \tag{26}$$

So, the characteristic field corresponding to $\sigma_2 = \frac{(1-h)u}{A}$ is also linearly degenerate.

Case 3 $\sigma_\pm = \frac{(1-h)u \pm a}{A}$

We have

$$\nabla \sigma_\pm = (\pm \frac{\gamma}{2a\rho A}, \mp \frac{a}{2\rho A}, \frac{(1-h)}{A}, -\frac{\sigma_\pm}{A}) \tag{27}$$

hence

$$\mathbf{r}_\pm \cdot \nabla \sigma_\pm = \pm \frac{\gamma + 1}{2a\rho A} \neq 0 \tag{28}$$

and the $\sigma_\pm$ characteristic fields are genuinely nonlinear.

3.2 Smooth Solution

The smooth solution from the $\sigma_\pm$ characteristic fields can be derived from the following system of ODE

$$\frac{d\rho}{dp} = \frac{1}{a^2} \tag{29}$$

$$\frac{du}{dp} = \pm \frac{1}{a\rho} \tag{30}$$

$$\frac{dA}{dp} = \mp \frac{h}{\rho a \sigma_\pm} \tag{31}$$

The solution for ρ, u, A relates the flow state $\mathbf{Q} = (p, \rho, u, A)^T$ in the rarefaction fan to the initial state $\mathbf{Q_0} = (p_0, \rho_0, u_0, A_0)^T$ upstream of the fan through the following expressions

$$\rho = \rho_0 (\frac{p}{p_0})^{1/\gamma} \tag{32}$$

$$u \mp \frac{2a}{\gamma - 1} = u_0 \mp \frac{2a_0}{\gamma - 1} \tag{33}$$

$$A = A_0 exp\left(\int_{p_0}^{p} \frac{\mp h dp}{a\rho((1-h)u \pm a)}\right) \tag{34}$$

To find the solution inside the rarefaction fan, we consider the characteristic ray through the origin $(0,0)$ and a general point (λ, ξ) inside the fan. The slope of the characteristic is

$$\frac{d\xi}{d\lambda} = \frac{\xi}{\lambda} = \sigma_{\pm} = \frac{(1-h)u \pm a}{A} \tag{35}$$

Making use of (32)-(34), eq.(35) becomes an equation for $p(\frac{\xi}{\lambda})$ as follows:

$$f(p) = \left(\frac{\gamma + 1 - 2h}{p_0^{\frac{\gamma-1}{2\gamma}}}\right) p^{\frac{\gamma-1}{2\gamma}} \mp 2(1-h) + \frac{\gamma - 1}{a_0}(1-h)u_0 \mp \frac{\gamma - 1}{a_0} A_0 \frac{\xi}{\lambda} exp(g(p)) = 0 \tag{36}$$

where

$$g(p) = \int_{p_0}^{p} \frac{\mp h dp}{a\rho((1-h)u \pm a)} \tag{37}$$

The other flow variables ρ, u and A as functions of $\frac{\xi}{\lambda}$ can be easily found from (32)-(34).

3.3 Discontinuous Solutions

We start from the Rankine-Hugoniot jump conditions of the system (24):

$$\sigma[\rho A] = [(1-h)\rho u] \tag{38}$$

$$\sigma[\rho u A] = [(1-h)\rho u^2 + p] \tag{39}$$

$$\sigma[\rho e A] = [(1-h)\rho u e + up] \tag{40}$$

$$\sigma[A] = -[hu] \tag{41}$$

where [.] denotes the jump across the discontinuity whose speed is denoted by $\sigma = \frac{d\xi}{d\lambda}$

Case 1: Shock Wave. We denote the pre-shock flow state by $\mathbf{Q_0} = (p_0, \rho_0, u_0, A_0)^T$ and the post shock flow state by $\mathbf{Q} = (p, \rho, u, A)^T$, respectively. Then the shock jump relations after some algebraic manipulations can be expressed in terms of $\alpha = \frac{p}{p_0}$ as follows:

$$\rho = \rho_0 \frac{\alpha(\gamma+1) + \gamma - 1}{\alpha(\gamma-1) + \gamma + 1} \tag{42}$$

$$u = u_0 \pm \frac{a_0}{\gamma}(\alpha - 1)\left(\frac{\frac{2\gamma}{\gamma+1}}{\alpha + \frac{\gamma-1}{\gamma+1}}\right)^{1/2} \tag{43}$$

$$A = A_0 - \frac{h(u-u_0)}{\sigma_{sh\pm}} \tag{44}$$

where

$$\sigma_{sh\pm} = \frac{(1-h)u_0}{A_0} \pm \frac{a_0}{A_0}\left(\frac{\gamma+1}{2\gamma}\alpha + \frac{\gamma-1}{2\gamma}\right)^{1/2} \tag{45}$$

Formulas (42)-(45) hold for $h : 0 \leq h \leq 1$.

Case 2: Slip line (a). For the slip line corresponding to the slope $\sigma_2 = \frac{(1-h)u}{A}$, from Rankine-Hugoniot jump conditions, (38)-(41), we find

$$u = u_0 \tag{46}$$

$$p = p_0 \tag{47}$$

$$A = A_0 \quad (if\ h \neq 1) \tag{48}$$

The only variable which can change its value freely across the slip line is the density ρ.

Case 3: Slip line (b). The other degenerate wave corresponds to the slope $\sigma_1 = 0$. From the Rankine-Hugoniot jump conditions we have

$$u = u_0 \tag{49}$$

$$p = p_0 \tag{50}$$

$$\rho = \rho_0 \quad (if\ h \neq 1) \tag{51}$$

The only variable which can change its value across this wave is A.

In the Lagrangian case when $h = 1$, $\sigma_1 = \sigma_2 = 0$, and the two slip lines coincide. In this case the jump relations across the slip line are

$$u = u_0 \tag{52}$$

$$p = p_0 \tag{53}$$

but ρ and A can jump arbitrarily.

4 The Shock-Adaptive Godunov Scheme

The only source of error in the Godunov scheme arises from averaging the flow quantities over a computational cell when representing the flow in all cells by piecewise constant states. While the error due to averaging is small in smooth flow regions and can be reduced by using a higher order schemes, e.g. MUSCL, it is large in cells containing discontinuities. As we noted earlier, for $h = 1$ the two slip lines coincide and we arrive at the Lagrangian formulation. In that case the slip line also coincides with a cell interface and the smearing effect induced by the averaging procedure across the slip line is thus avoided. In the case when two shocks intersect inside a cell, producing a slip line, we split the cell into two sub-cells with the slip line as cell interface; the smearing effect due to averaging across the slip line is thus also avoided. If we take advantage of this fact, then the only problem left is the shock resolution which can be dealt with by using a shock-adaptive Godunov scheme developed in [12] and [14] for steady supersonic flow. The results in [12] and [14] are excellent. Earlier, Harten and Hyman [20] had introduced the concept of a moving grid in order to resolve both slip line and shock wave simultaneously for 1-D unsteady Euler equations written in cartesian coordinates. But in trying to resolve both discontinuities they met some difficulties, especially in slip line resolution. In this paper the idea of Lepage and Hui [14] will be followed.

The basic idea of the shock-adaptive Godunov scheme consists of splitting of a **shock-cell**, i.e. a computational cell containing a shock wave, along the trajectory of the shock. The split shock-cell becomes two sub-cells: one entirely upstream of the shock and the other entirely downstream. In this way, the cell averaging procedure across the shock discontinuity, and the errors associated with it, are avoided, resulting in infinite shock resolution. The fictitious cell boundary separating the two sub-cells and moving through the regular grid at the local speed of the shock shall be called a **partition**. With this abstraction, the two sub-cells and the other (regular) cells can be treated on an equal footing in the Godunov scheme.

The shock-adaptive Godunov scheme is complemented by a shock-cell splitting criterion which triggers the splitting of a shock-cell in the presence of a shock in the flow field. In the approach considered here, a shock-cell is split if the pressure jump across an elementary shock wave, as obtained from the exact solution to the Riemann problem, is larger than some critical shock strength threshold, say if

$$\frac{p_u}{p_d} < \delta_{Shock}, \quad 0 < \delta_{Shock} < 1. \tag{54}$$

where the subscripts d and u refer to the downstream and upstream flow states, respectively. This desirable self-adaptivity feature permits for the automatic detection of a shock wave without a priori knowledge of its position nor its existence.

The value of $\delta_{Shock} = 1$ corresponds to splitting all cells along elementary shock waves, whereas $\delta_{Shock} = 0$ corresponds to no splitting and the scheme simply reduced to the classical Godunov scheme. In our calculations $\delta_{Shock} = 0.6$, corresponding to the entropy jump of 16%, was found to be satisfactory.

Now with the use of the shock-adaptive Godunov scheme in the Lagrangian coordinates, the errors arising from averaging across both discontinuities - shocks and slip lines - are avoided, and the numerical computation of unsteady flow needs be done only in the smooth flow regions. The utmost importance of the conservation form of the discretised equations [21] for the correct capturing of shocks is no longer necessary since shocks are now captured exactly, based on the information provided by the Riemann solutions. It is therefore possible to freely rewrite the governing equations in certain non-conservative form, which is advantageous, and for this purpose an entropy-conserving reformulation of the governing equations in the smooth flow region is proposed.

The motivation for the use of an alternative set of governing equations arises from the desire to eliminate the overshoots commonly observed in Lagrangian computation in the vicinity of slip lines (see Refs. 11 and 22; also Figures 3 and 8), despite the fact that in the case $h = 1$ the flow quantities are not averaged across a slip line.

Since the flow is isentropic along a pathline in a smooth flow region, the energy equa-

tion (the 3rd equation of (6)) can be replaced by the law of conservation of entropy.

$$\frac{\partial S}{\partial \lambda} = 0 \tag{55}$$

along a pathline, where $S = \frac{p}{\rho^\gamma}$. We note that the conservation law of entropy (55) applies only in regions of smooth flow, upstream or downstream of the shock. Across a shock discontinuity, the exact entropy jump is imposed by the shock-adaptive scheme through the splitting of the shock-cell.

5 The Unified Computer Code

With the Riemann solution given in section 3 and the shock-adaptive Godunov scheme explained in section 4, we are now in the position to describe the numerical procedure.

A pseudo-particle in the physical space marching in the flow direction of a fluid particle corresponds to a cell marching in the λ direction in the computational (λ, ξ) space. The superscript n refers to the marching time step number and the subscript i refers to the cell index number on a time line $\lambda = const.$

The following steps describe the numerical procedure of the shock-adaptive Godunov scheme upgraded by MUSCL. This scheme is applied only for $h = 1$ (Lagrangian coordinates). By putting the shock-detection parameter δ_{Shock} equal to zero (no cells are splitted) the described scheme reduces to the classical Godunov-MUSCL scheme, and it can then be applied for $0 \leq h \leq 1$.

Step 1. Initialisation at λ^0. Assume the initial conditions of a flow problem are given at $t = 0$ ($\lambda = 0$) in the physical space. Then a ξ-coordinate mesh is laid on the x line (for instance, we take ξ equal to be x) with

$$\xi = \xi_0, \xi_1, \xi_2, ..., \xi_m \tag{56}$$

Hence the flow variables $\mathbf{Q_i^0} = (p_i^0, \rho_i^0, u_i^0, A_i^0)$, $i = 1, 2, ..., m$, are known as initial conditions. Subsequently, $\mathbf{E_i^0}$ are available for all i, $i = 1, 2, ..., m$.

Step 2. Construction of interface fluxes. With all $\mathbf{E_i^n}$ and $\mathbf{Q_i^n}$ known at step n ($n = 0, 1, 2, ...$), the $\mathbf{Q}$ data are first upgraded or reconstructed via MUSCL procedure by nonlinear interpolation in the following way. Let f be any of the above variables p, ρ, u or A, then in the cell (i) and $(i+1)$, we assume linearly distributed states in both cells, and use nonlinear extrapolation to determine cell interface flow variables as follows:

$$f_r = f_{i+1} - 0.5(f_{i+2} - f_{i+1})\phi(r^+) \tag{57}$$

$$r^+ = \frac{f_{i+1} - f_i}{f_{i+2} - f_{i+1}} \tag{58}$$

$$f_l = f_i + 0.5(f_i - f_{i-1})\phi(r^-) \tag{59}$$

$$r^- = \frac{f_{i+1} - f_i}{f_i - f_{i-1}} \tag{60}$$

where $\phi(r) = max(0, min(1, r))$ is the minmod flux limiter and subscripts r and l correspond to the right and the left state, respectively. We emphasize that the MUSCL upgrading does not apply across shocks: the shocks are already captured exactly by the shock-adaptive Godunov scheme based on the Lagrangian coordinates, there is no room for further improvement by upgrading.

A local Riemann problem is solved at all cell interfaces, including partitions, for all adjacent cell pairs i and $i+1$. A Newton iterative method is employed (see [22]) for finding the values of pressure p^* and velocity u^* at the cell interface $\xi_{i+1/2}$. The numerical fluxes (see Appendix A)

$$(\Im^{\pm})_i^n = \begin{cases} \mathbf{F}(p_i^n, u_i^n) & \text{if } \pm\sigma_{i\pm1/2}^n < 0 \\ \mathbf{F}(p_{i\pm1/2}^*, u_{i\pm1/2}^*) + \sigma_{i\pm1/2}^n(\mathbf{E_i^n} - \mathbf{E_{i\pm1/2}^*}) & \text{if } \pm\sigma_{i\pm1/2}^n \geq 0 \end{cases} \tag{61}$$

are evaluated at $\xi_{i\pm1/2}$ where $\sigma_{i\pm1/2}^n$ are the slopes $d\xi/d\lambda$ of the interface $\xi_{i\pm1/2}$ at λ^n and $\mathbf{E_{i\pm1/2}^*}$ is the averaged conserved flow state along the inner (downstream) side of the shock relative to the shock-subcell being updated. The speeds $\sigma_{i\pm1/2}^n$ of the partitions are updated based on the speeds of the corresponding elementary shock waves in the local Riemann problems. The presence of a new shock is tested at all cell interfaces. If the splitting criterion is satisfied, a new partition is introduced to account for the incoming shock and the cell is split.

Step 3. Determination of the step size $\triangle\lambda^n$. To satisfy the stability condition of the scheme, the step size is determined as the minimum of the step sizes

$$\triangle\lambda^n = \frac{CFL}{\max_i \left\{ \frac{|\sigma^n_{i\pm 1/2}|}{\triangle\xi_i} \right\}} \tag{62}$$

for the regular cells and

$$\triangle\lambda^n = \min_i \left\{ \frac{\triangle\xi_i}{|\sigma^n_{i+1/2}| + |\sigma^n_{i-1/2}|} \right\} \tag{63}$$

for the shock-subcells which represents the intersection point of the $\pm$ waves in the shock-subcell, or equivalently, the intersection point of the incoming elementary wave with the opposing cell interface, also an elementary wave.

For an elementary rarefaction wave, $\sigma^n_{i\pm 1/2}$ is replaced by the speed of the leading Mach line (fastest characteristic). For an elementary shock wave, $\sigma^n_{i\pm 1/2}$ is replaced by the shock speed, since any disturbance propagating in the shock direction is bounded by the shock, with the flow upstream of the shock being undisturbed.

Step 4. Advancement of the average cell states from λ^n **to** $\lambda^{n+1} = \lambda^n + \triangle\lambda^n$**.** The average states $\mathbf{E}^{n+1}_i$ for all non-terminating cells, with domain

$$\{(\lambda,\xi) \in R^2 || \lambda^n < \lambda < \lambda^{n+1}, \xi^n_{i-1/2} + \sigma^n_{i-1/2}(\lambda - \lambda^n) < \xi < \xi^n_{i+1/2} + \sigma^n_{i+1/2}(\lambda - \lambda^n)\} \tag{64}$$

are obtained at λ^{n+1} using the difference equation

$$\mathbf{E}^{n+1}_i = \mathbf{E}^n_i - \frac{\triangle\lambda^n}{\triangle\xi^{n+1}_i}((\Im^+)^n_i - (\Im^-)^n_i) \tag{65}$$

with the composite fluxes given by (61). The cell width $\triangle\xi^{n+1}_i$ of a shock-subcell is updated using

$$\triangle\xi^{n+1}_i = \triangle\xi^n_i + (\sigma^n_{i+1/2} - \sigma^n_{i-1/2})\triangle\lambda^n \tag{66}$$

prior to advancing the conserved flow state. For a stationary coordinate slip line, $\sigma^n_{i+1/2} = 0$; for a partition, $\sigma^n_{i+1/2} = \sigma^n_{Shock}$, as obtained from the solution to the local Riemann problem. For a regular rectangular cell, the above difference equation reduces to the familiar updating formula used in the classical Godunov scheme.

Step5. Decoding to get $\mathbf{Q_i^{n+1}}$. The decode procedure is straightforward. From the expression for $\mathbf{E} = (e_1, e_2, e_3, e_4)^T$, where $e_1 = \rho A$, $e_2 = \rho A u$, $e_3 = \rho A e$ or $e_3 = \frac{p}{\rho^\gamma}$ (for shock-adaptive Godunov scheme) and $e_4 = A$, we have

$$u = \frac{e_2}{e_1} \tag{67}$$

$$\rho = \frac{e_1}{e_4} \tag{68}$$

$$p = \begin{cases} \left(\frac{e_3}{e_1} - \frac{u^2}{2}\right)(\gamma - 1)\rho, & h \neq 1 \\ e_3 \cdot \rho^\gamma, & h = 1 \quad (for\ shock - adaptive\ Godunov\ scheme) \end{cases} \tag{69}$$

$$A = e_4 \tag{70}$$

Step 6. Elimination of the terminating shock-subcells at λ^{n+1} (Only for shock-adaptive Godunov scheme). The shock-subcells terminating at λ^{n+1} are eliminated by removing the corresponding partitions and the upstream shock-subcells. This renders the downstream subcell a regular cell at λ^{n+1}.

Step7. Mapping results onto the physical space. To map results from computational space onto the physical space, trapezoidal integration is applied to get

$$x_i^{n+1} = x_i^n + 0.5 \cdot \triangle\lambda \cdot (hu_i^n + hu_i^{n+1}) \tag{71}$$

This step in the program is optional since the grid in the physical space does not participate in the computation; all computations are carried out in the transformed (λ, ξ) space. It is obvious that we will have some errors during mapping of computational results onto physical domain, but the errors are small as seen in the test examples.

Now the numerical procedure for advancing one time step is completed. To march forward further, one goes back to Step 2 and repeats Step 2-6.

6 Numerical Results and Comparisons

Six test problems from [23] and [24] and a piston problem [11] are selected to assess

the performance of the unified computer code and the effects of varying h on resolving flow discontinuities.

Test	ρ_l	u_l	p_l	ρ_r	u_r	p_r
1	5.99924	19.5975	460.894	5.99242	−6.19633	46.0950
2	1.0	0.0	1000.0	1.0	0.0	0.01
3	1.0	0.0	1.0	0.125	0.0	0.1
4	1.0	−2.0	0.4	1.0	2.0	0.4
5	0.445	0.699	3.528	0.5	0.0	0.571

Table 1: Initial data for 5 Riemann test problems

In all cases $\gamma = 1.4$ is used for the ratio of specific heats of the gas. Table 1 shows the data for the first five Riemann test problems in terms of primitive variables. In these tests the exact and numerical solutions are found in the spatial domain $0 \leq x \leq 2$, initial data consists of two constant states $\mathbf{Q_l} = (p_l, \rho_l, u_l, A_l)^T$ and $\mathbf{Q_r} = (p_r, \rho_r, u_r, A_r)^T$, separated by a discontinuity at $x = 1$, where $A_l = A_r = 1$. The numerical solutions are computed with $m = 100, 200, 400$ cells showing convergence to the exact solution. The results presented are those with $m = 200$ and the CFL number is 0.5. All the physical variables are discontinuous across a shock wave, but across a slip line only the density is discontinuous. For these cases, results for density ρ and specific internal energy $i = \frac{p}{(\gamma-1)\rho}$ are presented.

Test # 1

The solution of Test # 1 consists of three discontinuities: two shock waves and a slip line in between. They all travel to the right, and the left shock has a small positive speed. As we can see, in the Eulerian case (Figure 1), the left shock is sharply resolved. It was mentioned in [23] that slowly moving shocks are sharply resolved by Godunov's method, but there are some low frequency spurious oscillations in its vicinity, as we can see in the internal energy plot (Figure 1). The slip line in this case is badly smeared. The

resolution of the slip line is greatly improved with increasing h (Figures 2 and 3) and in the Lagrangian case ($h = 1$) the resolution of the both discontinuities is quite satisfactory, except that there are some undershoots and overshoots near the slip line (Figure 3). The shock-adaptive Godunov scheme perfectly resolves both types of discontinuities. (The results are presented in the physical and computational domain, Figure 4 and 5, respectively).

Test # 2

The solution to Test # 2 (the left half of the "Bang-bang" problem of Woodward and Colella [24]) consists of a left rarefaction, a slip line and a right shock. It has large pressure ratio and is not easy to compute accurately. The performance of the second-order Godunov scheme in the Eulerian case ($h = 0$) is seen to be quite poor (Figure 6): the resolution of discontinuities is worst for the slip line, the post shock value is not attained, and the internal energy plot gives a very smeared picture near the slip line. As we increase h to 0.5 the computed solution is getting closer to the exact solution (Figure 7), resolution of the slip line is much better than in Eulerian formulation. And for $h = 1$ (Lagrangian case) the resolution of both discontinuities is clear, although there are some overshoots near the slip line (Figure 8).

Again, as in Test # 1, the shock-adaptive Godunov scheme shows the best resolution of both discontinuities for Test # 2 (The results are presented in the physical and computational domain. Figure 9, Figure 10). The overshoots in the vicinity of the slip line are eliminated due to the use of the entropy conservative scheme, Eq.(55), and the behaviour of the computed solution in the rarefaction fan is also improved.

Test # 3

Test # 3 is the so called Sod test problem; its solution consists of a left rarefaction, a slip line and a right shock.

The slip line, seen in the density and internal energy plots, in Eulerian formulation is smeared over 12 cells (Figure 11). It is still smeared over about the same number of cells in case $h = 0.5$, but the computed solution near the slip line is a little closer to the

exact solution (Figure 12). We note that (Figure 13) the slip line is resolved crisply for $h = 1$ (Lagrangian case), but there are some overshoots and undershoots in the computed solution in it's vicinity. We further note that shock wave resolution is quite similar for all values of h. From Figures 14 and 15 we see that the perfect resolution of both shock wave and slip line is obtained by using shock-adaptive Godunov scheme ($h = 1$) with the use of entropy conservation, Eq.(55), in smooth flow regions. The overshoots and undershoots in the vicinity of the slip line in the density plot are eliminated. The attempt to resolve both shock and slip line in this case was done in [20], but was not satisfactory (see Figure 10 of [20]).

Test # 4

Test # 4, called the "123 problem", has a solution consisting of two strong rarefactions and a trivial stationary slip line. In this case none of the physical variables experience jump discontinuities. But it is interesting to see the behavior of the solution near the low density region. The performance of Godunov's method in this case is generally quite satisfactory even in Eulerian coordinates (Figure 16) as regards the physical variables, p, u and ρ, but not so for the specific internal energy ($i = \frac{p}{(\gamma-1)\rho}$) near the stationary slip line at $x = 1$, where both pressure and density are close to zero. Increasing h to $h = 0.5$ does not improve the accuracy (Figure 17). But the situation is improved in the Lagrangian formulation (Figures 18 and 19).

Test # 5

To further compare the performances of the shock-adaptive Godunov scheme with the self-adjusting grid method [20], we consider Test # 5, also called the Lax problem whose solution is easy to obtain computationally. Figure 20 shows reprinted results from [20]. The results for the same problem with the same conditions computed in Lagrangian formulation with shock-adaptive Godunov method are presented in the Figure 21. As we can see the resolution of the slip line as well as expansion wave is better in latter case.

Test # 6

This is an initial boundary value problem, the "Bang-bang" problem of Woodward and Colella [24], in which the gas is initially at rest in the region $0 < x < 1$ with pressure and density distributions as follows

$$\begin{cases} p = 1000.0, & \rho = 1.0 & (0 < x < 0.1) \\ p = 0.01, & \rho = 1.0 & (0.1 \leq x < 0.9) \\ p = 100.0, & \rho = 1.0 & (0.9 \leq x < 1.0) \end{cases}$$

It is a most challenging problem for Eulerian computations, and [24] had to use, in most cases, more than 3,000 cells plus further grid refinements near the slip lines. In our computation using shock-adaptive Godunov scheme based on Lagrangian coordinates, we use 400 uniform cells in the ξ space and the results for velocity and density at different times are plotted in Figures 22 and 23, respectively, together with the corresponding results of Woodward and Colella for comparison. The computed results (dots) are connected by solid lines to better illustrate the positions of discontinuities.

It is seen that our results for shock and slip line resolution are crispy and are just as good as [24]. Figure 24 shows a comparison of results using 400 cells and 800 cells. It is seen that the latter results have better resolution in the smooth flow region and are about the same as [24]. We note in passing, that a recent Eulerian computation [25, Fig.11b,c] produces smeared slip lines, as expected.

Piston problem

This problem is set up to test the performance of the code for initial boundary-value problem with a moving boundary. It is well-known that a shock wave will be formed gradually in most cases when the piston is pushing inside the gas at rest. However, we may also determine the motion of a piston $\Gamma : x = X(t)$ towards a gas such that a shock wave of finite strength is formed suddenly in the interior of the flow field and, consequently, a slip line and a rarefaction are also generated. Here, we set out to determine the family of such piston paths. A similar problem was studied by Hui and Loh [11] for steady supersonic flow. We shall follow their idea.

Assume the fluid be aligned on the positive x-axis direction initially. Let $P_0(t_0, x_0)$ be the point where the shock of finite strength is first formed. Then, clearly, every straight line joining P_0 to a point $P(t, x(t))$ on Γ is a Mach line of the flow. Hence

$$x_0 - x = \left(a_0 + \frac{\gamma+1}{2}\frac{dx}{dt}\right)(t_0 - t) \tag{72}$$

Solving the above ordinary differential equation yields,

$$x - a_0 t_0 = \frac{2a_0}{\gamma - 1}(t_0 - t) + k(t_0 - t)^{\frac{2}{\gamma+1}} \tag{73}$$

and the integration constant k can be determined from the initial condition $x(0) = 0$. Here, we get $k = -a_0\left(\frac{\gamma+1}{\gamma-1}\right)t_0^{\frac{\gamma-1}{\gamma+1}}$. After some simplifications we have the following result

$$x(t) = \frac{\gamma+1}{\gamma-1}a_0 t_0\left(1 - \frac{2t}{(\gamma+1)t_0} - (1 - \frac{t}{t_0})^{\frac{2}{\gamma+1}}\right) \tag{74}$$

where a_0 is the speed of sound of the undisturbed gas. In our case the path of the piston is given as follows: the piston moves according to the above equation up to some time $t_s < t_0$ and then it moves with constant speed equal to its speed at the time $t = t_s$. (we take $t_s = 0.7$ in our calculations).

Numerically the initial boundary-value problem with a moving boundary posts a challenging problem in Eulerian computation. If we change the system of cartesian coordinates to a system moving with the piston, the difficulty due to the presence of a moving boundary is avoided, but a new difficulty appears: in the transformed system it is difficult to apply Godunov scheme because the equations of the Riemann problem now have variable coefficients and may not admit similarity solutions. Alternatively, we may refine the grid near the piston path during its motion, which itself is not a simple task but it then introduces additional errors in the computational results. The latter way was used in our computation. With Lagrangian formulation ($h = 1$) all these difficulties disappear. Now, the boundary condition is very easy to apply, because the moving boundary is a coordinate line, and the Godunov scheme is easily applied.

Here we present some of the results computed in Lagrangian and Eulerian formulation. The solution is sketched in the $x - t$ plane in Figure 25. After the shock, the slip line and

the expansion fan have emerged at $t = t_0$ and $x = a_0 t_0$, the expansion fan reflects from the piston, goes through the slip line and interacts with the shock wave producing entropy, as can be seen in the plots at time $t = 3.0$. (Figures 31 and 32) The major difficulty arising is that the numerical solution at the singular point $t = t_0$, $x = a_0 t_0$, where the shock is suddenly formed, is contaminated, meaning the numerical shock is spread over many cells. When we carry on our computation, we observe that even in the Lagrangian case ($h = 1$) the slip line is not perfectly resolved - it is spread over roughly the same number of computational cells (see Figures 28, 30, 32). But this number of cells never increases during further marching in time. In the Eulerian case the number of cells across the slip line increases with time (Figures 27,29 and 31). In order to test the performance of the code, theoretical results were introduced at time t_0 when the shock is formed. With these, the computational results (using shock-adaptive Godunov scheme) at the times $t > t_0$ are perfect. These results with $\triangle\xi = 0.001$ are therefore taken as the exact results for comparison. Figure 26 shows the comparison between the results obtained by shock-adaptive Godunov scheme in Lagrangian formulation with $\triangle\xi = 0.01$ and $\triangle\xi = 0.001$. As we can see they are practically the same. Figures 27-32 show the performance of the solutions obtained in Eulerian and Lagrangian formulations at different times. From these plots we conclude that the resolution of the slip line as well as shock is better in Lagrangian formulation. The latter is due to the fact that computational cells, literally fluid particles, are compressed inside the computational region yielding better resolution of the discontinuities.

7 Conclusions

Effects of coordinates on the numerical computation of one-dimensional unsteady inviscid flow are systematically investigated by using a unified coordinate system and by varying the speed hu of the pseudo-particle from $h = 0$ (Eulerian) to $h = 1$ (Lagrangian).

From comparisons in the seven test problems, it is concluded that while shock resolution is independent of h, the Lagrangian coordinates give best accuracy and resolution of slip lines (or contact lines). Furthermore, with the use of shock-adaptive Godunov scheme based on Lagrangian coordinates, infinite shock resolution can also be achieved. It is therefore recommended that one-dimensional unsteady flow be best computed using the shock-adaptive Godunov scheme based on Lagrangian coordinates. In this regard, we note pleasantly that it was Lagrangian coordinates that were used in the two classical pioneering papers on shock-capturing by Von Neumann and Richtmyer [26] and by Godunov [27].

However, we point out [19] that the situation is quite different for two-dimensional (unsteady or steady) flow, for which the Lagrangian system of coordinates is deficient and definitely not the best. Rather, the unified coordinates with h determined by preserving grid angles have been shown to produce best results.

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Appendix A

Here we derive the form of the numerical fluxes given by eq.(61). Let us consider two

cells, i and $i+1$, with partition between them having the slope $\frac{d\xi}{d\lambda} = \sigma^n_{i+1/2} > 0$, Figure 33. (The case $\sigma^n_{i+1/2} < 0$ can be derived similarly). Applying the divergence theorem to the cells i and $i+1$, we obtain:

$$\begin{aligned}
\triangle\xi_i^{n+1}\mathbf{E_i^{n+1}} &= \triangle\xi_i^n\mathbf{E_i^n} + \sigma^n_{i+1/2}\cdot\triangle\lambda\cdot\mathbf{E^*_{i+1/2}} - \triangle\lambda\cdot(\mathbf{F}(p^*_{i+1/2},u^*_{i+1/2}) - \mathbf{F}(p^*_{i-1/2},u^*_{i-1/2}))\\
\triangle\xi_{i+1}^{n+1}\mathbf{E_{i+1}^{n+1}} &= \triangle\xi_{i+1}^n\mathbf{E_{i+1}^n} - \sigma^n_{i+1/2}\cdot\triangle\lambda\cdot\mathbf{E^n_{i+1}} - \triangle\lambda\cdot(\mathbf{F}(p^*_{i+3/2},u^*_{i+3/2}) - \mathbf{F}(p^n_{i+1},u^n_{i+1}))
\end{aligned}$$

where $\mathbf{E^*_{i+1/2}}$ is the averaged conserved flow state along the inner (downstream) side of the shock having speed $\sigma^n_{i+1/2}$. Using $\triangle\xi_i^{n+1} = \triangle\xi_i^n + \sigma^n_{i+1/2}\cdot\triangle\lambda$ and $\triangle\xi_{i+1}^{n+1} = \triangle\xi_{i+1}^n - \sigma^n_{i+1/2}\cdot\triangle\lambda$, the above equations can be written in the form

$$\begin{aligned}
\mathbf{E_i^{n+1}} &= \mathbf{E_i^n} - \frac{\triangle\lambda}{\triangle\xi_i^{n+1}}\left(\mathbf{F}(p^*_{i+1/2},u^*_{i+1/2}) + \sigma^n_{i+1/2}\cdot(\mathbf{E_i^n} - \mathbf{E^*_{i+1/2}}) - \mathbf{F}(p^*_{i-1/2},u^*_{i-1/2})\right)\\
\mathbf{E_{i+1}^{n+1}} &= \mathbf{E_{i+1}^n} - \frac{\triangle\lambda}{\triangle\xi_{i+1}^{n+1}}\left(\mathbf{F}(p^*_{i+3/2},u^*_{i+3/2}) - \mathbf{F}(p^n_{i+1},u^n_{i+1})\right)
\end{aligned}$$

reproducing the numerical fluxes of eq.(61).