Journal of Computational Physics **180,** 110–119 (2002)
doi:10.1006/jcph.2002.7078

A Note on the Unified Coordinate System for Computing Shock Waves[1]

Zi-Niu Wu[2]

Department of Engineering Mechanics, Tsinghua University, Beijing 100084, People's Republic of China

Received June 7, 2001; revised April 8, 2002

In 1999 [*J. Comput. Phys.* **153**, 596], Hui and his co-workers proposed a unified coordinate system for computing compressible flows with discontinuous solutions. In their coordinate system, there is a free parameter h such that the traditional Eulerian approach and Lagrangian approach correspond to the particular cases $h = 0$ and $h = 1$, respectively. Hence this approach unifies the two classical methods for describing fluid flows. In this note we consider a one-dimensional problem and we show that there is a parameter range within $0 < h < 1$, such that the coordinate transformation is not invertible across a shock wave. In addition, there is a value of h such that the transformation becomes singular. Hence the parameter h should be restricted to a value close to 0 or 1 near a shock wave. This restriction does not occur away from a shock wave. This note clearly shows that the unified coordinate system of Hui *et al.* involves interesting properties that should be considered in practical applications.

Key Words: unified coordinate system; shock wave; invertibility condition; singularity.

1. INTRODUCTION

In classic fluid mechanics, there are two traditional approaches to describing fluid flows: the Eulerian approach and the Lagrangian approach. In the Eulerian approach, one considers what happens at every fixed point in space as a function of time. The velocities and the other properties of fluid elements are considered to be functions of time and fixed-space coordinates. In the Lagrangian approach, one looks for the dynamic history of each selected fluid element. The positions of fluid particles and the other properties are considered to be functions of the time and their initial positions. Both approaches have some advantages in

[1] This work was supported by Chinese National Natural Science Foundations (Contract 10025210) and by the China NKBRSF project (Contract 2001CB409600).

[2] Fax: 86-10-62773794. E-mail: ziniuwu@tsinghua.edu.cn.

0021-9991/02 $35.00

classic fluid mechanics [16]. They are regarded as equivalent to each other [19] except that the Lagrangian approach gives more information by telling each fluid particle's history.

The greatest disadvantage of the Eulerian approach is that fluid particles move across cell interfaces. It is this convective flux that causes excessive numerical diffusion in the numerical solutions. As a result, discontinuities such as shock waves and slip lines (contact discontinuities) are smeared out, although there are exceptions, such as the standard Roe scheme for a steady shock.

The Lagrangian approach, which is used by a wide community [1, 5, 9], needs the use of a moving frame and uses fluid particles as computational cells. Consequently, there is no convective flux across cell boundaries and the numerical diffusion can be minimized.

Recently, Hui and his co-workers proposed a unified coordinate system which unifies both approaches [4, 6–8]. This unified approach combines the advantages of the Eulerian approach and the Lagrangian approach. It involves a free parameter h which is allowed to vary with position (see [4, 6–8] for more details for the choice of h). The traditional Eulerian and Lagrangian approaches correspond to the particular cases $h = 0$ and $h = 1$, respectively. An equation for h can also be derived to ensure some quality requirement of the grid system. Note that the unified coordinate approach is different from other kinds of unified Lagrangian–Eulerian approaches, such as the arbitrary Lagrangian–Eulerian (ALE) approach [2, 13, 14].

In this short note we consider whether h can be allowed to vary arbitrarily within the range $0 < h < 1$. This note is restricted to the one-dimensional Euler equations in gas dynamics and to the case of continuous h. The Euler equations, in the original coordinate system (x, t), can be written in the conservative form

$$w_t + f(w)_x = 0, \tag{1}$$

with

$$\begin{aligned} w &= (\rho, \rho u, \rho E)^t, \\ f(w) &= \left(\rho u, \rho u^2 + p, \rho u\left(E + \frac{p}{\rho}\right)\right)^t. \end{aligned}$$

Here ρ is the density, u is the velocity of the fluid particle, E is the total energy,

$$p = (\gamma - 1)\left(\rho E - \frac{1}{2}\rho u^2\right)$$

is the pressure, and γ is the ratio between the specific heats at constant pressure and constant volume. The sound speed is defined by $a = \sqrt{\gamma p/\rho}$.

Let w_l and w_r be the left and right states of the discontinuity. We use $\langle w\rangle = w_r - w_l$ to denote the jump across the discontinuity. Then in the physical space the Rankine–Hugoniot relation [3, 15]

$$\langle f(w)\rangle = s'\langle w\rangle, \quad x = x_s, \tag{2}$$

where x_s denotes the position of the discontinuity and $s' = \frac{dx_s}{dt}$ is the speed of the shock wave, is satisfied for both shock wave and contact discontinuity.

We only consider the case that the shock wave has a positive speed, i.e., $s' > 0$. The case with $s' < 0$ can be symmetrically considered.

There are two cases: the left-going shock wave and the right-going shock wave. Here left and right mean relative to the fluid upstream of the shock.

For a left-going shock wave, the fluid crosses the shock from the left, i.e., $u_l > s'$; in which case the entropy condition, which states that the relative flow upstream (on the left of the shock) must be supersonic, requires $u_l - s' > a_l$. Hence, a physically relevant left-going shock wave satisfies the condition

$$s' < u_l - a_l. \tag{3}$$

For a right-going shock wave, the fluid crosses the shock from the right so that $u_l - s' < 0$ (the fluid velocity relative to the shock is negative on both sides). In this case, the entropy condition requires the relative flow downstream (on the left-hand side) of the shock to be subsonic, i.e., $u_l - s' > -a_l$. Hence, a physically relevant right-going shock wave satisfies the condition

$$u_l < s' < u_l + a_l. \tag{4}$$

Let $M = u_l/a_l$ be the Mach number. Using the classic Rankine–Hugoniot relation [3, 10–12, 15, 17], we have

$$\frac{u_r}{u_l} = \frac{1}{M}\frac{s'}{a_l} + \frac{(\gamma - 1)\left(M - \frac{s'}{a_l}\right)^2 + 2}{(\gamma + 1)\left(M - \frac{s'}{a_l}\right)M}, \tag{5}$$

$$\frac{p_r}{p_l} = \frac{2\gamma\left(M - \frac{s'}{a_l}\right)^2}{\gamma + 1} - \frac{\gamma - 1}{\gamma + 1}. \tag{6}$$

For a given p_l, the pressure p_r must be positive. This requires, by (6), the following inequality to be satisfied:

$$s' < u_l - a_l\sqrt{\frac{\gamma - 1}{2\gamma}} \quad \text{or} \quad s' > u_l + a_l\sqrt{\frac{\gamma - 1}{2\gamma}}. \tag{7}$$

Note that for $\gamma > 1, 0 < \sqrt{\frac{\gamma-1}{2\gamma}} < 1$. Combining (3), (4), and (7), we note that to ensure the entropy condition and positivity condition, the speed of a shock wave with $s' > 0$ should satisfy the condition

$$0 < s < M - 1 \quad \text{or} \quad M + \sqrt{\frac{\gamma - 1}{2\gamma}} < s < M + 1, \tag{8}$$

where

$$s = \frac{s'}{a_l} = \frac{M}{u_l}s' \tag{9}$$

is the relative shock speed.

2. UNIFIED COORDINATE SYSTEM AND INVERTIBILITY CONDITION

The unified coordinate system (ξ, τ) invented by Hui and his co-workers [4] is related to the original coordinate system (x, t) by

$$dt = d\tau, \tag{10}$$

$$dx = A d\xi + B d\tau, \tag{11}$$

where B is related to the fluid velocity u by

$$B = hu \tag{12}$$

and A must satisfy the Cauchy–Riemann relation (called geometrical conservation laws)

$$\frac{\partial A}{\partial \tau} = \frac{\partial B}{\partial \xi}. \tag{13}$$

Note that $dt = d\tau$ does not necessarily mean $t = \tau$. Moreover, the use of the notation τ avoids possible loss of terms while performing derivation.

Following Hui *et al.* [4], the frame derivative is defined by

$$\frac{D_B \xi}{Dt} = \xi_t + B\xi_x.$$

It can be shown that $\frac{D_B \xi}{Dt} = 0$ so that B is the speed of the moving frame.

Still using (10) and (11), we have

$$A = x_\xi = \xi_x^{-1}.$$

Hence A is the Jacobian of the coordinate transformation.

Invertibility condition. For the transformation to be invertible, we must impose

$$A > 0. \tag{14}$$

Following Viviand [18], system (1) in the transformed frame can be written in the conservative form (called physical conservation law by Hui *et al.* [4])

$$W_\tau + F(W)_\xi = 0, \tag{15}$$

with

$$W = Aw,$$

$$F(W) = A(\xi_t w + \xi_x f).$$

The physical conservation law (15) and the geometric conservation law (13) are solved simultaneously in the unified coordinate system approach.

Across a shock wave, not only the physical conservation law but also the geometric conservation law must satisfy the Rankine–Hugoniot relation. Now consider the jump relation in the transformed space (ξ, τ). If (15) is self-contained, then the Rankine–Hugoniot jump relation is

$$\langle F(W)\rangle = \sigma\langle W\rangle, \quad \xi = \xi_s, \tag{16}$$

where ξ_s is the position of the discontinuity and σ is the speed of discontinuity in the transformed space.

Introducing $W = Jw$ and $F(W) = J(\xi_t w + \xi_x f)$ into (16), and noting that $J = A$ and $\xi_t = -\frac{B}{A}$, we obtain from (16)

$$\langle -Bw + f\rangle = \sigma\langle Aw\rangle. \tag{17}$$

PROPOSITION 1. *If A satisfies the Rankine–Hugoniot relation*

$$\langle -B\rangle = \sigma\langle A\rangle, \tag{18}$$

then the jump relation in the physical space (2) *and the jump relation in the transformed space* (17) *are equivalent*, *with σ given by*

$$\sigma = \frac{s' - B_l}{A_l}. \tag{19}$$

Proof. The left-hand side of (17) can be expanded as

$$\langle -Bw + f\rangle = -\langle Bw\rangle + \langle f\rangle = -\langle B\rangle w_r - \langle w\rangle B_l + \langle f\rangle \tag{20}$$

and the right-hand side of (17) can be expanded as

$$\sigma\langle Aw\rangle = \sigma\langle A\rangle w_r + \sigma\langle w\rangle A_l. \tag{21}$$

Inserting (20) and (21) into (17) yields

$$-\langle B\rangle w_r - \langle w\rangle B_l + \langle f\rangle = \sigma\langle A\rangle w_r + \sigma\langle w\rangle A_l,$$

and thus the following relation holds:

$$\langle f\rangle = (B_l + \sigma A_l)\langle w\rangle + (\sigma\langle A\rangle + \langle B\rangle)w_r.$$

Applying relation (19) to the above relation leads to

$$\langle f\rangle = s'\langle w\rangle + (\sigma\langle A\rangle + \langle B\rangle)w_r,$$

which, with A subjected to the constraint (18), yields exactly the jump relation (2).

From (18), we have, for continuous h,

$$A_r = A_l\left(1 + \frac{B_l - B_r}{s' - B_l}\right) = A_l\left(1 + \frac{h(u_l - u_r)}{s' - hu_l}\right) = A_l\left(1 + \frac{h\left(1 - \frac{u_r}{u_l}\right)}{\frac{s}{M} - h}\right). \tag{22}$$

When h is discontinuous, the second equality in the above equation should be modified as

$$A_r = A_l\left(1 + \frac{h_l u_l - h_r u_r}{s' - h_l u_l}\right)$$

and the subsequent analysis could be continued by adding a jump $\triangle h$ to $h_l = h$ so that $h_r = h_l + \triangle h$. If we note the relative jump by $r = \triangle h/h$, then the third equality in (22) can be replaced by

$$A_r = A_l\left(1 + \frac{h\left(1 - (1+r)\frac{u_r}{u_l}\right)}{\frac{s}{M} - h}\right). \tag{23}$$

One can repeat the subsequent analysis to consider the role of r. This is, however, beyond the objective of the current note, which is restricted to continuous h. In fact h may be required to vary discontinuously only in high dimensions, as will be noted more clearly at the end of this note.

Using the jump relation (5) for velocity, expression (22) can be rewritten as

$$A_r = A_l\left[1 + h\left(\frac{M - s - \frac{(\gamma-1)(M-s)^2+2}{(\gamma+1)(M-s)}}{s - hM}\right)\right]. \tag{24}$$

In consequence, the invertibility condition (14) can be expressed as

$$S(h) = 1 + h\left(\frac{M - s - \frac{(\gamma-1)(M-s)^2+2}{(\gamma+1)(M-s)}}{s - hM}\right) > 0. \tag{25}$$

3. CONDITION OF NONINVERTIBILITY

From (25), we have

$$S(0) = 1 \tag{26}$$

and

$$S(1) = \frac{(\gamma-1)(M-s)^2 + 2}{(\gamma+1)(M-s)^2} > 0. \tag{27}$$

Hence the invertibility condition (14) is satisfied for the classic Eulerian approach ($h = 0$) and the classic Lagrangian approach ($h = 1$).

Now let us see if there are values of $h \in (0, 1)$ such that $S(h) < 0$. Since $S(0) > 0$ and $S(1) > 0$, $S(h)$ can be negative if there is a point $h = h_a$ at which $S(h) = 0$ and $\frac{dS(h)}{dh} \neq 0$. Setting $S(h_a) = 0$ yields

$$h_a = \frac{(\gamma+1)(M-s)s}{((\gamma-1)M + 2s)(M-s) + 2} \tag{28}$$

and

$$\frac{dS(h_a)}{dh} = \frac{2(M-1-s)(M+1-s)}{(\gamma+1)(M-s)\left(-s+s\frac{(\gamma+1)(M-s)}{((\gamma-1)M+2s)(M-s)+2}M\right)^2}. \tag{29}$$

Obviously, the inequality $\frac{dS(h_a)}{dh} \neq 0$ holds if

$$s \neq M-1 \quad \text{and} \quad s \neq M+1. \tag{30}$$

Now we want to look for the condition such that h_a defined by (28) satisfies $0 < h_a < 1$. Obviously, $h_a > 0$ only if

$$0 < s < M. \tag{31}$$

To look for the condition such that $h_a < 1$, we rewrite (28) as

$$h_a = \frac{1}{\frac{(\gamma-1)\frac{M}{s}+2}{(\gamma+1)} + \frac{2}{(\gamma+1)(M-s)s}}.$$

Under (31), we have

$$\frac{(\gamma-1)\frac{M}{s}+2}{(\gamma+1)} > 1,$$

so that

$$h_a < \frac{1}{1+\frac{2}{(\gamma+1)(M-s)s}} < 1.$$

Conditions (30) and (31) can be combined as

$$0 < s < M, \quad s \neq M-1 \tag{32}$$

However, we must only consider a physically relevant shock wave, for which constraint (8) must be fulfilled. Combining (32) and (8), we obtain

PROPOSITION 2. *If the speed of a physically relevant shock wave, with* $s > 0$, *satisfies the constraint*

$$0 < s < M-1, \tag{33}$$

then the function $S(h)$ *becomes negative around* $h = h_a$, *where* h_a, *given by* (28), *satisfies the condition*

$$0 < h_a < 1.$$

In other words, there is a parameter range $h \in (0, 1)$ *such that the transformation* (10)–(11) *is not invertible.*

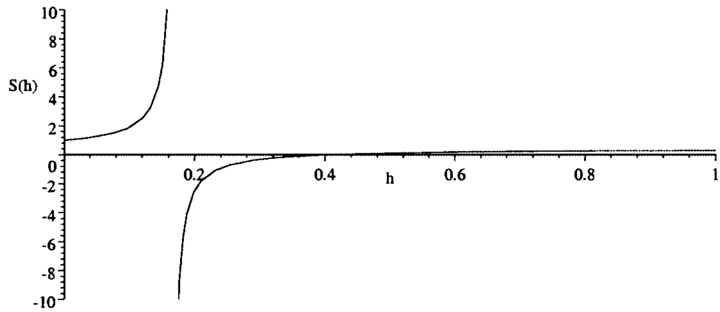

FIG. 1. Function $S(h)$ for $s = 0.5$ and $M = 3$.

4. MORE DETAILS AND DISCUSSIONS

The function $S(h)$ is singular for some h satisfying $0 < h < 1$. To see that, let us put $S(h_b)^{-1} = 0$. Then we obtain

$$h_b = \frac{s}{M}. \tag{34}$$

Obviously, $0 < h_b < 1$ for s satisfying (32).

A further analysis shows that for $0 < s < M - 1$, we have $h_a > h_b$; that is, the singularity point is at the left of the zero point.

Let us consider $s = 0.5$ and $M = 3$ so that condition (33) is satisfied (the function $S = S(h)$ is displayed in Fig. 1). Hence for $h \in (0.167, 0.4)$, $S(h) < 0$.

Now consider $s = 1.5$ and $M = 1.2$ so that condition (33) is not satisfied (the function $S = S(h)$ is displayed in Fig. 2). Here we always have $S(h) > 0$.

In summary, we have the following conclusions.

1. If the flow is such that condition (32) is not satisfied, then the unified coordinate system works well. Recall that s is the shock speed normalized by the sound speed at the left-hand side of the shock wave.

2. If condition (32) is satisfied, then necessarily we have a range of h lying inside (0, 1) such that $S(h) < 0$. According to (26) and (27), $S(h)$ has finite and positive values at $h = 0$ and $h = 1$. This means that there exists two positive values δ_1 and δ_2 such that the transformation is invertible for $h \in (0, \delta_1)$ and $h \in (1 - \delta_2, 1)$. Also, δ_1 and δ_2 are large

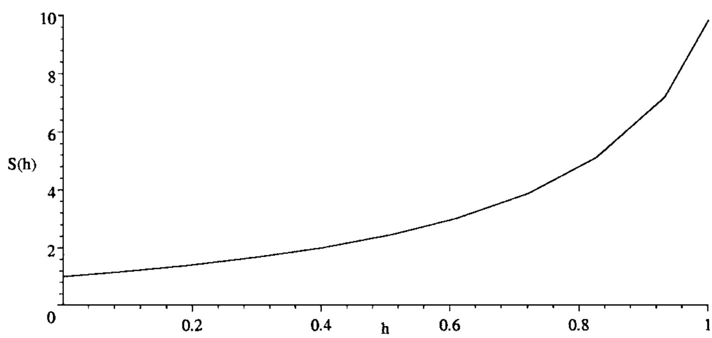

FIG. 2. Function $S(h)$ for $s = 1.5$ and $M = 1.2$.

enough so that the unified coordinate system works well for a large range of h around 0 or 1.

3. If one insists on letting the value h vary in (0, 1), one just needs to ensure that h is close to 0 or 1 across a shock wave. For smooth-flow regions and for contact discontinuities, the above phenomena does not occur, so there is no restriction on h. However, near a shock wave, one can simply use a value h close to 0 or 1, since there are good numerical methods for both the Eulerian approach and the Lagrangian approach to give sharp resolution of shock waves.

5. FURTHER PROBLEMS

There are two further questions which arise from high-dimensional problems.

The first is whether the current results hold exactly true for high dimensions, though intuition might tell us that it holds true since 1-D is a particular case of 2-D or 3-D. The 2-D or 3-D case is more complex while we note that Ref. [4] did not report any difficulty in the 2-D computation. A possible reason would be that in the direction normal to the shock, it happened that h did not lie in the range leading to negative $S(h)$. This issue will be considered when we consider high-dimensional problems in the future.

The second question is related to the continuity of h. In [4] h is controlled locally by preserving the grid angle in 2-D and the resulting equation for h is solution dependent. Since the solution is discontinuous across a shock wave, h might be discontinuous, too. If h is discontinuous, then the second equality (22) does not hold true and the conclusions could be slightly different. It is doutful that the equation for h can be solved analytically. Even with tremendous effort it is unlikely that one can arrive at conclusions as fundamental as for the currect 1-D study.

ACKNOWLEDGMENTS

The author wishes to thank Professor W. H. Hui (Department of Mathematics, Hong Kong University of Science and Technology) for many helpful discussions of this work. The comments by both referees were also helpful in achieving the final version of the paper. Notably, one referee pointed out an error in the selection of physically relevant shock waves.

REFERENCES

1. M. S. Hall, A comparision of first and second order rezoned and Lagrangian Godunov solutions, *J. Comput. Phys.* **90**, 458 (1990).
2. C. W. Hirt, A. A. Amsden, and J. L. Cook, An arbitrary Lagrangian–Eulerian computing method for all flow speeds, *J. Comput. Phys.* **14**, 227 (1974).
3. H. Hugoniot, Sur la propagation du movement dans les corps et spécialement dans les gas parfaits, *J. Ecole Polytech.* **57**, 1 (1887).
4. W. H. Hui, W. P. Li, and Z. W. Li, A unified coordinate system for solving the two-dimensional Euler equations, *J. Comput. Phys.* **153**, 596 (1999).
5. W. H. Hui and C. Y. Loh, A new Lagrangian method for steady supersonic flow computation, Part 1, *J. Comput. Phys.* **89**, 207 (1990); Part 2, **103**, 450 (1992); Part 3, **103**, 465 (1992).
6. W. H. Hui and S. Koudriakov, The role of coordinates in the computation of discontinuities in one-dimensional flow, *CFD J.* **8**, 495 (2000).
7. W. H. Hui and S. Koudriakov, A unified coordinate system for solving the three-dimensional Euler equations, *J. Comput. Phys.* **172**, 235 (2001).

8. W. H. Hui and S. Koudriakov, Computation of the shallow water equations using the unified coordinates, *SIAM J. Sci. Comput.* **27**, 1615 (2002).
9. M. S. Liou, An extended Lagrangian method, *J. Comput. Phys.* **118**, 294 (1995).
10. H.-O. Kreiss and J. Lorenz, *Initial-Boundary Value Problems and the Navier–Stokes Equations* (Academic Press, San Diego, 1989).
11. P. Lax, Hyperbolic systems of conservation laws and the mathematical theory of shock waves, in *Conference of the Board of Mathematics and Science* (Soc. for Industr. & Appl. Math., Philadelphia, 1973), Vol. II.
12. P. Lax, Weak solutions of nonlinear hyperbolic equations and their numerical computation, *Commun. Pure Appl. Math.* **7**, 159 (1954).
13. L. G. Margolin, Introduction to "An arbitrary Lagrangian–Eulerian computing method for all speeds," *J. Comput. Phys.* **135**, 198 (1997).
14. W. Pracht, Calculating three-dimensional fluid flows at all speeds with an Eulerian–Lagrangian computing mesh, *J. Comput. Phys.* **17**, 132 (1975).
15. W. J. M. Rankine, On the thermodynamic theory of waves of finite longitudinal disturbance, *Philos. Trans. R. Soc.* **160**, 277 (1870).
16. B. K. Shivamoggi, *Theoretical Fluid Dynamics* (Wiley, New York, 1998).
17. J. Smoller, *Shock Waves and Reaction-Diffusion Equations* (Springer-Verlag, Berlin/New York, 1994).
18. H. Viviand, Formes conservatives des equations de la dynamique des gaz, *Rech. Aerosp.* **1**, 65 (1974).
19. D. H. Wagner, Equivalence of Euler and Lagrangian equations of gas dynamics for weak solutions, *J. Differential Eq.* **68**, 118 (1987).