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Evaluation of rotated upwind schemes for contact discontinuity and strong shock

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Abstract

Rotated upwind schemes have been evaluated as carbuncle-free shock-capturing methods. In order to reveal the relation between the rotated upwind-differencing direction and the performance of rotated upwind schemes, theoretical and numerical investigations are made. Three commonly used upwind schemes, including Roe scheme, AUSM⁺ scheme and Van Leer scheme are investigated. According to the theoretical analysis, the dissipative terms of each upwind scheme are changed by the rotation procedure. Especially, the dissipative density term in the numerical flux function of rotated upwind schemes introduces extra dissipation. The numerical cases include simulations of laminar boundary layer, steady twin vortices and strong shock. The numerical results show that the carbuncle phenomenon can be eliminated by rotated upwind schemes, and the contact resolving capability of rotated upwind schemes is deteriorated by the rotation procedure. Monotonicity of the dissipation with rotation angle is also shown in the numerical results. Therefore, a novel rotation strategy that defines the rotation angle by a pressure weight function is introduced for tuning the dissipative effects adaptively. This strategy shows not only carbuncle-free result in hypersonic inviscid flow simulations, but also accurate results in viscous flow simulations.

Keywords: rotated upwind scheme; carbuncle phenomenon; shock-capturing; dissipative density term; contact discontinuity; rotation strategy

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1. Introduction

Hypersonic flow simulations are very challenging due to shock instabilities, such as carbuncle phenomenon [1], odd-even decoupling [2] and so on. In general, shock instabilities are more prominent and complicate in multidimensional simulations [3, 4].

5 Researches have shown that the shock instabilities are closely related to the resolution of contact discontinuity and shear wave. Liou [5] analysed the mechanism of numerical diffusivity of several numerical flux schemes. He suggested that the dissipative pressure term would be a key factor for shock stability. Pandolfi and D'Ambrosio [6] suggested that the carbuncle phenomenon affects flux-difference-splitting (FDS)

10 schemes that explicitly take into account the presence of contact surface. In fact, for an upwind scheme, research suggested that strict stability and exact resolution of contact discontinuity are not compatible [7]. Therefore, devise a combined upwind scheme [8] or a tunable dissipation would be a practical strategy for acquiring shock stability and contact resolution at the same time. Quirk [2] suggested that using combined fluxes,

15 then a dissipative flux can be used in the shock regions. In contrast, in stead of a different upwind scheme, second-order artificial dissipation could be directly added on a flux-vector-splitting (FVS) method [9] in the shock regions [10, 11].

Because shock instabilities are multidimensional numerical phenomena, some researches have taken the multidimensional effects as a critical factor for the construction

20 of numerical fluxes. The rotated Riemann solver, as one type of the multidimensional upwind methods [12], was showing an alterable dissipation that can be adaptively activated to suppress shock instability [13]. As one of the pioneer works, in order to lessen the dependence between numerical solution and grid orientation, Levy et al [12] examined a "rotated Riemann solver" by exploiting the multidimensional nature of the

25 governing equations. Several physical meaningful directions were used as the direction for upwind differencing. In Levy's work, the approximate Riemann solver of Roe [14] was implemented to calculate fluxes in both the upwind direction and its perpendicular direction, thus the rotated scheme requires additional computation resources over grid-aligned schemes. Besides the efficiency issue, the choice of the upwind differencing

30 direction and the combination of upwind schemes were investigated by subsequent

researches.

Ren [13] presented a rotated Roe scheme which is free from shock instabilities. In Ren's work, the upwind-differencing direction was defined as the direction of the velocity-difference vector across each grid interface. The dissipation properties of the rotated flux function was theoretically analysed. Different from Ren's work, Nishikawa and Kitamura [15] combined Roe scheme and HLL scheme [16] for eliminating shock instabilities. Thereinto, a fewer-wave solver (HLL) was automatically applied in the direction normal to the shocks, and then shock instabilities will be suppressed. A full-wave solver (Roe) was applied across shear layers to avoid an excessive amount of dissipation. In Nishikawa and Kitamura's work, simulations of supersonic jet and flat plate boundary layer were conducted for the demonstration of the shear layers resolving capability. Zha et al [17] used ECUSP scheme [18, 19] instead of Roe scheme for the flux solution in the direction parallel to the shocks. Huang et al [20] managed to resolve the problem of the numerical shock instabilities in HLLC solver [21], and one of their method was the rotated HLLC scheme.

After all these works, problems still exist. For example, flat plate boundary layer simulation has been commonly used for evaluating the contact and shear layer resolving capability of upwind schemes. However, rotated upwind schemes usually become a grid-aligned scheme (rotate to the face normal direction) in the flat plate boundary layer simulation. The problem is, even in a shock-free simulation, velocity difference vector direction (or the other specific upwind-differencing directions) is not always parallel or perpendicular to the normal direction of interface. Furthermore, in order to acquire a full convergence, the upwind-differencing direction vector was suggested to be freezed after an order of magnitude reduction of the residuals [15]. In other words, the actual upwind-differencing direction does not strictly coincide with the suggested flow features. Therefore, it is necessary to investigate the relation between the dissipation property and rotation angle of rotated upwind schemes specifically.

In this paper, rotated upwind schemes are investigated based on former researches. The numerical mass flux, which was investigated by Liou [5] and well utilized by Kim et al [22], is used for analysing the performance of rotated schemes. The presented paper is organized as follows. In the next section, a finite volume formulation of the

governing equations is given. In section 3, basic concepts of rotated upwind schemes are presented, as well as the basic rotation strategy applied in this paper. Theoretical analyses are introduced in section 4. Numerical experiments are presented in section 5 to further clarify the conclusions in section 4. Then the new rotation strategy could be proposed straightforwardly, as presented in section 6. Finally, the paper ends with the conclusions.

2. Finite Volume Discretization

Consider the two-dimensional compressible Navier-Stokes equations,

$$\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial (\mathbf{F}_c - \mathbf{F}_v)}{\partial x} + \frac{\partial (\mathbf{G}_c - \mathbf{G}_v)}{\partial y} = \mathbf{0}. \quad (1)$$

The viscous fluxes $\mathbf{F}_v$ and $\mathbf{G}_v$ are solved by a central scheme for unstructured grid [23]. The viscous fluxes, of which the solution method is not investigated in this work, will be omitted for simplicity. Then the simplified equations become the Euler equations. The conservative variables and convective fluxes are

$$\mathbf{U} = \begin{bmatrix} \rho \\ \rho u \\ \rho v \\ \rho E \end{bmatrix}, \mathbf{F}_c = \begin{bmatrix} \rho u \\ \rho u^2 + p \\ \rho uv \\ \rho uH \end{bmatrix}, \mathbf{G}_c = \begin{bmatrix} \rho v \\ \rho uv \\ \rho v^2 + p \\ \rho vH \end{bmatrix}, \quad (2)$$

where ρ is the density, u and v are the velocity components in the x and y directions respectively, and p is the static pressure. The specific total energy E and enthalpy H are given by

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

$$H = \frac{\gamma}{\gamma - 1} \frac{p}{\rho} + \frac{1}{2} (u^2 + v^2), \quad (4)$$

where $\gamma = 1.4$ for calorically perfect gas. Consider the cell-centered finite volume discretization, the computation domain is discretized to a set $\{I\}$ of quadrilateral and/or triangular cells. For each cell $i \in \{I\}$, have a set of faces $\{K_i\}$. Each face $k \in \{K_i\} \cap \{K_j\}$ connects two neighbouring cells i and j . The cell-residual $\mathbf{Res}_i$ is defined as a

numerical approximation of the integral over the cell of the spatial operator divided by the cell area S_i , that is

$$\mathbf{Res}_i = - \sum_{k \in \{K_i\}} \Phi_k(\mathbf{n}_k) \Delta s_k / S_i, \quad (5)$$

where the Δs_k is the length of cell face $k \in \{K_i\}$, $\mathbf{n}_k$ is the unit vector outward normal to that face, and $\Phi_k(\mathbf{n}_k)$ is the numerical flux, which is a numerical approximation to $[\mathbf{F}_c, \mathbf{G}_c] \cdot \mathbf{n}_k$. The cell-averaged value $\bar{\mathbf{U}}_i$ is then evolved by the residual as

$$\frac{\partial \bar{\mathbf{U}}_i}{\partial t} = \mathbf{Res}_i, \quad (6)$$

which is integrated in time by the Forward-Euler method, Runge-Kutta method or LU-SGS method.

The numerical flux $\Phi_k(\mathbf{n}_k)$ is evaluated by using the left and right states of the interface. If the cell-averaged values are taken as the left and right states, the accuracy of the numerical method will be first-order in space. In order to achieve second-order accuracy, Gauss-Green method [24] is applied to calculate the cell gradient $\nabla \bar{\mathbf{U}}_i$. Therefore, the left and right states of face k are

$$\begin{aligned} \bar{\mathbf{U}}_k^L &= \bar{\mathbf{U}}_i + \phi_i \nabla \bar{\mathbf{U}}_i \cdot (\mathbf{x}_k - \mathbf{x}_i), \\ \bar{\mathbf{U}}_k^R &= \bar{\mathbf{U}}_j + \phi_j \nabla \bar{\mathbf{U}}_j \cdot (\mathbf{x}_k - \mathbf{x}_j), \end{aligned} \quad (7)$$

where $i, j \in \{I\}$, and $k \in \{K_i\} \cap \{K_j\}$. In the following numerical investigations, the slope limiter of Venkatakrishnan [25] is used for the calculation of ϕ in second-order spatial accuracy supersonic flow simulations. Otherwise, the limitation value ϕ is simply set as 1.

As mentioned by Ren [13], the rotated methods that use the same set of face data in every direction are efficient and can be easily extended to higher order of accuracy by using spatial interpolations or reconstructions. In this paper, the rotated schemes would be extended to second-order accuracy by the above formula, and thus the limiter can also be replaced by the other commonly used methods.

3. Basics of rotated upwind schemes

Reconsider Eq.1 in a numerical discretized form. The numerical flux $\Phi_k(\mathbf{n}_k)$ across each face k can be determined by solving the one-dimensional Euler equations in the

direction of vector $\mathbf{n}_k$. The equations are

$$\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \Phi_k}{\partial \mathbf{n}_k} = \mathbf{0}. \quad (8)$$

In what follows, the subscript k is omitted for simplicity.

The rotated upwind schemes are based on the decomposition of direction $\mathbf{n}$ into two orthogonal directions $\mathbf{n}_1$ and $\mathbf{n}_2$,

$$\mathbf{n} = C_1 \mathbf{n}_1 + C_2 \mathbf{n}_2, \quad \mathbf{n}_1 \cdot \mathbf{n}_2 = 0, \quad (9)$$

where $\mathbf{n}_1$ and $\mathbf{n}_2$ are unit vector, $C_1 = \mathbf{n}_1 \cdot \mathbf{n}$ and $C_2 = \mathbf{n}_2 \cdot \mathbf{n}$. In order to keep the same left and right states in both directions, $\mathbf{n}_1$ and $\mathbf{n}_2$ are chosen to make $C_1 \geq 0$ and $C_2 \geq 0$. Therefore, the numerical flux is then decomposed into the following form,

$$\Phi(\mathbf{n}) = C_1 \Phi(\mathbf{n}_1) + C_2 \Phi(\mathbf{n}_2). \quad (10)$$

The decomposition of $\mathbf{n}$ into two vector $\mathbf{n}_1$ and $\mathbf{n}_2$ is purely a geometrical procedure. The physical features of flow field could be taken into account to determine the choices of $\mathbf{n}_1$ and $\mathbf{n}_2$. Usually, the vector $\mathbf{n}_1$ stands for some physically meaningful direction. For example, Ren [13] suggested that it would be effective and robust for Roe solver to align $\mathbf{n}_1$ with the velocity-difference vector between two adjacent cells,

$$\mathbf{n}_1 = \begin{cases} \mathbf{n}, & \text{if } \|\Delta \mathbf{V}\| \leq \varepsilon, \\ \frac{\Delta \mathbf{V}}{\|\Delta \mathbf{V}\|}, & \text{otherwise,} \end{cases} \quad (11)$$

where $\Delta \mathbf{V}$ is the velocity-difference vector, ε is a predesigned small threshold, and then $\mathbf{n}_2$ is given as

$$\mathbf{n}_2 = \frac{(\mathbf{n}_1 \times \mathbf{n}) \times \mathbf{n}_1}{\|(\mathbf{n}_1 \times \mathbf{n}) \times \mathbf{n}_1\|}. \quad (12)$$

However, in this paper, the upwind differencing direction is defined in a different way. The decomposition of $\mathbf{n}$ is defined as

$$\mathbf{n}_1 = \mathbf{T}_1 \mathbf{n}, \quad \mathbf{n}_2 = \mathbf{T}_2 \mathbf{n}, \quad (13)$$

$$\mathbf{T}_1 = \begin{bmatrix} \cos(\alpha) & \sin(\alpha) \\ -\sin(\alpha) & \cos(\alpha) \end{bmatrix}, \quad \mathbf{T}_2 = \begin{bmatrix} \cos(\alpha - \pi/2) & \sin(\alpha - \pi/2) \\ -\sin(\alpha - \pi/2) & \cos(\alpha - \pi/2) \end{bmatrix},$$

where α is the rotation angle at each interface. Therefore, the rotation could be controlled by defining the angle, and the effects of different rotation angles could be more observable. The detail of the designation of rotation angle will be introduced in section

85 6.

4. Analyses

The relation between the numerical mass flux and the shock stability or contact resolving capability was investigated theoretically and numerically by Liou [5]. Liou suggested that the existed pressure contribution to numerical mass fluxes will be the
90 root for causing shock instabilities. Somewhat differently, Pandolfi and D'Ambrosio [6] suggested that the carbuncle phenomenon should be connected to those solutions of the Riemann problem that explicitly take into account the contact surface. Based on Liou's theorem, Kim et al [22] analysed and improved Roe scheme. Most importantly for the presented work, Kim et al proved that the perturbation introduced by the pres-
95 sure term in the numerical mass flux function could be damped by a proper dissipative density term. So far, although debates and investigations are still carrying on the mechanism of shock instability, the method of Liou has proved to be helpful for analysing and improving the performance of upwind schemes.

An investigation on the dissipative terms of rotated upwind schemes is briefly per-
100 formed in this section. The analysis method of Liou and Kim et al is adopted here. Following paragraphs first introduce the fluxes of Roe scheme, AUSM⁺ (Advection Upwind Splitting Method) scheme [26] and Van Leer scheme [27]. Noteworthily, the Roe scheme was deemed as a carbuncle-prone scheme, the AUSM⁺ scheme was considered as a light-carbuncle-prone scheme and the Van Leer scheme has been evaluated
105 as a carbuncle-free scheme [6]. Subsequently, the flux function of each rotated upwind scheme is investigated by comparing with its grid-aligned counterpart.

4.1. Numerical mass fluxes of grid-aligned upwind schemes

Based on the grid-aligned formulation, the numerical flux in Eq.8 can be written as a split form [5, 22]. Thereinto, the numerical mass flux is rewritten as

$$\Phi_{1/2}^{(\rho)} = \frac{1}{2}[(\rho V_n)_L + (\rho V_n)_R] - \frac{1}{2}[D^{(\rho)}\Delta\rho + D^{(V_n)}\Delta V_n + D^{(p)}\Delta p], \quad (14)$$

where $V_n = [u, v] \cdot \mathbf{n}$, $D^{(\rho)}$, $D^{(V_n)}$ and $D^{(p)}$ are functions of mean quantities $\bar{\mathbf{U}}(\mathbf{U}_L, \mathbf{U}_R)$, and the difference operator is $\Delta(\bullet) = (\bullet)_R - (\bullet)_L$. Because of their effects on the performance of upwind schemes, $D^{(\rho)}$ and $D^{(p)}$ will be investigated in the following paragraphs. The flux function of each grid-aligned scheme will be shown as follows.

For Roe scheme, the numerical flux could be written as [26]

$$\Phi_{1/2} = \frac{1}{2}[(V_n\Phi)_L + (V_n\Phi)_R - |\hat{\mathbf{A}}|\Delta\mathbf{U} + \mathbf{P}_L + \mathbf{P}_R], \quad (15)$$

$$\Phi_{L,R} = \begin{bmatrix} \rho \\ \rho u \\ \rho v \\ \rho H \end{bmatrix}_{L,R}, \quad \mathbf{P}_{L,R} = \begin{bmatrix} 0 \\ n_x p \\ n_y p \\ 0 \end{bmatrix}_{L,R}, \quad (16)$$

$$|\hat{\mathbf{A}}|\Delta\mathbf{U} = |\Delta\hat{\Phi}|_1 + |\Delta\hat{\Phi}|_2 + |\Delta\hat{\Phi}|_3 + |\Delta\hat{\Phi}|_4. \quad (17)$$

The over hat in the formulas means the variables are Roe's averaged approximations.

In Eq.17, the terms in the RHS are represented as follows,

$$|\Delta\hat{\Phi}|_1 = |\hat{V}_n|(\Delta\rho - \frac{\Delta p}{\hat{a}^2}) \begin{bmatrix} 1 \\ \hat{u} \\ \hat{v} \\ \frac{\hat{u}^2 + \hat{v}^2}{2} \end{bmatrix}, \quad |\Delta\hat{\Phi}|_2 = |\hat{V}_n|\hat{\rho}(n_y\Delta u - n_x\Delta v) \begin{bmatrix} 0 \\ n_y \\ -n_x \\ \hat{u}n_y - \hat{v}n_x \end{bmatrix},$$

$$|\Delta\hat{\Phi}|_{3,4} = |\hat{V}_n \pm \hat{a}|(\frac{\Delta p \pm \hat{\rho}\hat{a}\Delta V_n}{2\hat{a}^2}) \begin{bmatrix} 1 \\ \hat{u} \pm n_x\hat{a} \\ \hat{v} \pm n_y\hat{a} \\ \hat{H} \pm \hat{a}\hat{V}_n \end{bmatrix}. \quad (18)$$

Therefore, the dissipative terms in the numerical mass flux of Roe scheme are [5, 22]

$$\begin{aligned} D^{(\rho)} &= |\lambda_2|, \\ D^{(p)} &= (|\lambda_1| + |\lambda_3| - 2|\lambda_2|)/2\hat{a}^2, \end{aligned} \quad (19)$$

where $\{\lambda_k, k = 1, 2, 3\} = \{\hat{V}_n - \hat{a}, \hat{V}_n, \hat{V}_n + \hat{a}\}$, $\hat{a}$ is the speed of sound.

For AUSM⁺ scheme, the numerical flux is written as [26]

$$\Phi_{1/2} = \frac{1}{2}a_{1/2}[M_{1/2}(\Phi_L + \Phi_R) - |M_{1/2}|(\Phi_R - \Phi_L)] + P_{1/2}, \quad (20)$$

where the subscript 1/2 is not an average of left and right states, but rather a weighted function. Therefore, the dissipative terms of AUSM⁺ scheme are [5]

$$\begin{aligned} D^{(\rho)} &= |a_{1/2}M_{1/2}| = |V_{1/2}|, \\ D^{(p)} &= 0, \end{aligned} \quad (21)$$

where $M_{1/2} = \mathcal{M}_{(\beta)}^+(M_L) + \mathcal{M}_{(\beta)}^-(M_R)$ is the surface mach number, left and right Mach numbers are defined as $M_{L,R} = (V_n)_{L,R}/a_{1/2}$, $a_{1/2}$ is defined by Liou [26].

The Van Leer scheme, which is a typical FVS scheme, could be written as

$$\Phi_{1/2} = \Phi_L + \Phi_R, \quad (22)$$

where $\Phi_{L,R}$ were defined by van Leer [27] and different from Eq.16. While $|M| < 1$, the mass flux of Van Leer scheme is

$$\Phi_{L,R}^{(\rho)} = \pm \left[\frac{\rho a}{4} (M \pm 1)^2 \right]_{L,R}. \quad (23)$$

Therefore, according to Eq.14, the dissipative terms of Van Leer scheme are written as [5]

$$\begin{aligned} D^{(\rho)} &= a_L \mathcal{M}_{(0)}^+(M_L) - a_R \mathcal{M}_{(0)}^-(M_R), \\ D^{(p)} &= 0, \end{aligned} \quad (24)$$

115 where $M_{L,R} = (V_n)_{L,R}/a_{L,R}$.

The split functions in Eq.21 and Eq.24 are defined here to facilitate the discussion:

$$\mathcal{M}_{(\beta)}^\pm(M) = \begin{cases} \frac{1}{2}(M \pm |M|), & \text{if } |M| \geq 1, \\ \pm \frac{1}{4}(M \pm 1)^2 \pm \beta(M^2 - 1)^2; & -1/16 \leq \beta \leq 1/2, \text{ otherwise.} \end{cases} \quad (25)$$

The parameter β is set to meet the requirements on monotonicity, consistency and continuously differentiability of the split function [26]. For the AUSM⁺ scheme, β is usually set as 1/8. For the Van Leer scheme, β is always equal to zero.

4.2. Numerical mass fluxes of rotated upwind schemes

The terms $D^{(\rho)}$ and $D^{(p)}$ have proved to be critical factors for the performance of upwind schemes. Thereinto, the exact solution for a contact discontinuity moving with speed u_c requires that [5]

$$D^{(\rho)} = |u_c|, \quad \text{as } (u, p)_L = (u, p)_R = (u_c, p) \text{ and } \rho_L \neq \rho_R. \quad (26)$$

120 This criterion is fulfilled in the Roe scheme and AUSM⁺ scheme, and these two schemes possess contact resolving capability. But the Van Leer scheme has proved to be inaccurate for the solution of contact discontinuity by both numerical cases and the above criterion. In the following paragraphs, the rotated upwind schemes will be examined on the above criterion.

125 Because the mass fluxes are linearized about the dissipative terms, which are scalar, following results are presented. It should be noticed again that the C_1 and C_2 in the following equations will not be smaller than zero by the proper choices of $\mathbf{n}_1$ and $\mathbf{n}_2$.

For the rotated Roe scheme,

$$\begin{aligned} D_n^{(\rho)}|_A &= |\lambda_2|_n = |\hat{V}_n| = |C_1 \hat{V}_{n_1} + C_2 \hat{V}_{n_2}| \\ &\leq C_1 |\hat{V}_{n_1}| + C_2 |\hat{V}_{n_2}| = C_1 |\lambda_2|_{n_1} + C_2 |\lambda_2|_{n_2} \\ &= C_1 D_{n_1}^{(\rho)} + C_2 D_{n_2}^{(\rho)} = D_n^{(\rho)}|_R, \end{aligned} \quad (27)$$

where the subscript A denotes the grid-Aligned scheme, and the subscript R denotes the Rotated scheme. Obviously, $D_n^{(\rho)}|_A$ is different from $D_n^{(\rho)}|_R$, and the criterion Eq.26
130 is not fulfilled in the rotated Roe scheme. Therefore, the rotated Roe scheme could not show exact solutions for contact discontinuity. Furthermore, based on Eq.27, the difference between the grid-aligned Roe scheme and the rotated Roe scheme could vary with the rotation angle, even if the local velocity is not changed.

For the rotated AUSM⁺ scheme, similar to Eq.27, the dissipative density term shows following relation,

$$\begin{aligned} D_n^{(\rho)}|_A &= |V_{1/2}|_n = |C_1 (V_{1/2})_{n_1} + C_2 (V_{1/2})_{n_2}| \\ &\leq C_1 |V_{1/2}|_{n_1} + C_2 |V_{1/2}|_{n_2} \\ &= C_1 D_{n_1}^{(\rho)} + C_2 D_{n_2}^{(\rho)} = D_n^{(\rho)}|_R. \end{aligned} \quad (28)$$

Therefore, the rotation effects of the rotated AUSM⁺ scheme are expected to be similar
 135 to those of the rotated Roe scheme.

For the rotated Van Leer scheme, we simplify the formula by assuming the problem
 is in subsonic flow condition. Therefore,

$$D^{(\rho)} = \frac{1}{4}[a_L(M_L + 1)^2 + a_R(M_R - 1)^2]. \quad (29)$$

For a stationary contact discontinuity in which $u_c = 0$, both the grid-aligned and rotated
 Van Leer schemes are showing $D^{(\rho)} \geq 0$. In a rotation framework, the speed of sound
 remains the value of the grid-aligned calculation. It is easily deduced that

$$C_1(M_{L,R} + 1)_{n_1}^2 + C_2(M_{L,R} + 1)_{n_2}^2 \geq (M_{L,R} + 1)_n^2. \quad (30)$$

Therefore, $D_n^{(\rho)}|_R$ will be larger than $D_n^{(\rho)}|_A$. It is expected that the rotated Van Leer
 scheme is more dissipative than the grid-aligned Van Leer scheme.

The dissipative pressure terms of AUSM⁺ scheme and Van Leer scheme are always
 equal to zero in both the grid-aligned and rotated frameworks. On the contrary, the
 140 term $D^{(p)}$ is not equal to zero in both the grid-aligned and rotated Roe scheme. Based
 on the conjecture of Liou, $D^{(p)} \neq 0$ is the root for causing the shock instabilities [5].
 Although this conjecture has been challenged, to eliminate the $D^{(p)}$ term was regarded
 as an important part for improving the shock stability [22, 28, 4]. In the following
 sections, the actual performance of each upwind scheme will be examined by a serial
 145 of numerical cases.

5. Numerical cases and discussions

The numerical cases are designed to test the performance of rotated upwind schemes
 in both the strong shock stability and contact resolving capability. Therefore, numeri-
 cal simulations of flat plate laminar boundary layer flow, subsonic viscous flow around
 150 a cylinder and inviscid hypersonic flow around a cylinder are conducted.

5.1. Case 1: Flat plate laminar boundary layer

The simulation of laminar boundary layer flow over a flat plat is usually used as
 a standard test for the accuracy of viscous flux formulations. Here, grid-aligned and
 rotated upwind schemes are investigated by a serial of simulations.

155 The simulations are performed by Roe scheme, AUSM⁺ scheme, Van Leer scheme and their rotated versions. Free stream Mach number is 0.3, Reynolds number is 10^6 . In order to reveal the effects of the rotation on upwind differencing direction, the results of rotated upwind schemes in three predefined rotation angles $\alpha = 4.5^\circ, 22.5^\circ, 45^\circ$ are compared with those of the grid-aligned schemes and the Blasius' result.

160 The flow field is discretized into a quadrilateral grid, the height of the first layer of cells at the non-slip wall is 0.0001, the aspect ratio of the grid cell that in the front of the flat plate is 1. All the computations use LU-SGS scheme for temporal integration, the CFL number of which is 10^6 . Computations are deemed to be converged by 10 orders of magnitude reduction in the density residual. Velocity profiles across the boundary
165 layer are compared. In order to present a common standard of diffusive results, the result of the grid-aligned Van Leer scheme is also presented along with the results of Roe and AUSM⁺ schemes.

Figure 1: Grid for laminar boundary layer flow simulations

In Fig.2, the Roe scheme is investigated. Obviously, the grid-aligned Roe scheme shows accurate result, but the rotated Roe schemes present dissipative results. There-
170 into, the result of the rotated Roe ($\alpha = 22.5^\circ$) scheme is similar to that of the Van Leer scheme, and the rotated Roe ($\alpha = 45^\circ$) scheme is more dissipative than the Van Leer scheme. Therefore, the rotation angles of the rotated Roe schemes significantly affects the contact resolution, and the dissipation will be more significant if the rotation angle becomes larger.

175 The AUSM⁺ scheme presents accurate velocity profile, which is similar to the result of Roe scheme. However, dissipative results are presented by the rotated AUSM⁺ schemes. According to these results, rotation angle is an important factor for the accu-

Figure 2: Velocity profile of laminar boundary layer flow: Roe and rotated Roe schemes

Figure 3: Velocity profile of laminar boundary layer flow: AUSM⁺ and rotated AUSM⁺ scheme

racy of boundary layer resolution. It should be noted that the rotated AUSM⁺ schemes are more dissipative compared with the rotated Roe schemes.

180 In Fig.4, the grid-aligned Van Leer scheme shows inaccurate result, which is already shown in Fig.2 and Fig.3. Furthermore, the rotated Van Leer schemes are more dissipative compared with the grid-aligned scheme. This is supporting the analyses in subsection 4.2.

In general, the boundary layer resolution of upwind schemes will be deteriorated

Figure 4: Velocity profile of laminar boundary layer flow: Van Leer and rotated Van Leer schemes

185 by the rotation on upwind differencing directions. The estimations for the velocity of contact discontinuity are inaccurate, as introduced in section 4, and thus the deteriorated accuracy of the rotated upwind schemes could be easily predicted. However, the monotonicity of the dissipation with rotation angle, as has been shown in this section, will be a basic standpoint in this paper.

190 5.2. Case 2: Subsonic viscous flow around a cylinder

In the previous case, the rotation angles of the upwind differencing direction are predefined without consideration on local flow directions. In flat plate boundary layer flow, the streamlines are mostly conformed with grid lines and the flow gradients are approximately changing in one direction. Therefore, it is necessary to investigate the rotated upwind schemes in a more complicate flow field. Furthermore, the high aspect-ratio grid, which is used for the simulations of the dominant flow features in the former cases, might causes complicate numerical viscous effects [29]. In order to thoroughly investigate the dissipative effects of the rotated upwind schemes, two-dimensional subsonic flow around a cylinder [30] is simulated. In this case, the flow features are more complicate and the most part of the flow field is discretized by isotropic cells.

200 The simulations are performed on an O-type quadrilateral grid, as shown in Fig.5. The free stream Mach number is 0.3 and Reynolds number is 40. The diameter of the

cylinder is 1, the height of first layer of cells is 0.001. All the computations use the LU-SGS scheme of which the maximum CFL is 100, and the density residuals of the
205 computations are reducing 10 order of magnitudes. Three definitions of upwind differencing directions are applied in this case. The first one is using 0 degree rotation angle, which leads to the grid-aligned scheme. The second one is the 45 degree angle rotated scheme, which is denoted as the MR (Maximum Rotation) scheme for simplicity in the following paragraphs. In the last definition, the directions for the convective fluxes
210 computations are exactly accordance of the coordinate directions of two-dimensional plane, thus the scheme is isolated with grid geometry. The last scheme is denoted as CA (Coordinate Aligned) scheme.

Figure 5: Grid for the simulation of subsonic flow around a cylinder

For brevity, only the streamlines in the results of the grid-aligned and rotated Roe schemes are visually shown in Fig.6. The lengths of the calculated closed wakes are
215 presented in Table 1. Here, the exactness of the calculated wakes will be used as the estimation of the simulation accuracy. In general, the MR schemes present the smallest separated wake, which means the dissipation is significant.

The grid-aligned Roe scheme shows accurate result in the simulation. Obviously,

Figure 6: Streamlines of subsonic flow around cylinder. (a) Roe E-fix. (b) Roe CA. (c) Roe MR.

two rotated Roe schemes show poor accuracy. Especially, the Roe MR scheme shows
 220 inaccurate result which is similar to the result of Van Leer scheme. The variation
 tendencies of the dissipation of the rotated AUSM⁺ schemes and rotated Van Leer
 schemes are the same as that of the rotated Roe schemes. It could be found that, the
 more significant rotation apply, the more dissipative result will show. Therefore, the
 monotonicity of the dissipation of rotated schemes with rotation angle is also held
 225 in multidimensional cases. Rotation procedure on upwind schemes will substantially
 deteriorate the resolution of contact discontinuity and eventually disperse the viscous
 flow features.

Table 1: Lengths of the closed wakes

		Grid-Aligned	Coordinate-Aligned	Maximum Rotation
Experiment	2.13	–	–	–
Roe	–	2.135	2.095	1.925
AUSM ⁺	–	2.097	2.044	1.849
Van Leer	–	1.922	1.869	1.659
Roe WR-M	2.132	–	–	–

5.3. Case 3: Inviscid hypersonic flow around a cylinder

Last two cases show the behaviours of the rotated upwind schemes in the simulations for viscous flows. In order to investigate the shock stability of the rotated schemes, this subsection is presented.

Inviscid hypersonic flow around a cylinder is a well-known test case to invoke or examine the catastrophic carbuncle failings of some upwind schemes. In this section, the free stream Mach number is set as 20. This test problem is computed on a quadrilateral grid with 80 cells in the radial direction, 120 cells in the circumferential direction, and a unstructured triangular grid with 12156 cells. Boundary nodes of each grid are halved in Fig.7 for the clarity of observation, and inner nodes/cells are lessened correspondingly.

Second-order spatial accuracy could be easily acquired by applying the formula of Eq.7. Whereas, in second-order spatial accuracy hypersonic flow simulations, the computation results could be affected by both the upwind scheme and the slope limiter. Therefore, although improvements are also shown in the second-order accuracy simulations, only the first-order results of the presented numerical cases are shown. The Forward-Euler temporal scheme is applied with CFL= 0.5. Note that the entropy fix [31] with parameter $\delta = 0.2$ is only implemented in the original grid-aligned Roe scheme.

Firstly, the computation results of the grid-aligned schemes on quadrilateral grid are presented in Fig.8. A typical carbuncle phenomenon can be found in the result of Roe scheme. In fact, the Roe scheme could be showing shock instability in a Mach

Figure 7: Grids for simulations of inviscid hypersonic flow around a cylinder (boundary nodes are halved in the figures for clarity).

number smaller than 3. In contrast, Van Leer scheme presents perfect density contour
 lines. Slight anomalies are found in the result of $AUSM^+$ scheme. A zigzag-shaped
 shock wave that similar to the result of Shima et al [32] and folded contour lines in the
 stagnation point are shown. These results (or similar results) are already given by other
 researches. Secondly, Fig.9 presents the results that computed on the triangular grid.
 Obviously, $AUSM^+$ scheme shows carbuncle phenomenon as well as Roe scheme, but
 Van Leer scheme presents carbuncle-free result (even not as perfect as the result on
 quadrilateral grid). The result of $AUSM^+$ scheme further support the conclusion that
 $AUSM^+$ scheme could be denoted as a "Light carbuncle prone scheme" [6]. Finally,
 the results of the MR schemes are presented in Fig.10. Roe MR scheme, $AUSM^+$ MR
 scheme and Van Leer MR scheme are all showing carbuncle-free results.

Liou [5] suggested that the non zero dissipative pressure term should be the root of
 shock instabilities. Therefore, the grid-aligned $AUSM^+$ scheme and Van Leer scheme
 should be showing carbuncle-free results in the simulations. However, the $AUSM^+$
 scheme, which shows accurate boundary-layer resolution, is unstable in the simulation

Figure 8: Inviscid hypersonic flow around a cylinder at $M = 20$ (grid-aligned solvers on quadrilateral grid). Thirty equally spaced contour lines from $\rho = 1$ to $\rho = 8$.

Figure 9: Inviscid hypersonic flow around a cylinder at $M = 20$ (grid-aligned solvers on triangular grid). Thirty equally spaced contour lines from $\rho = 1$ to $\rho = 8$.

Figure 10: Inviscid hypersonic flow around a cylinder at $M = 20$ (rotated solvers on triangular grid). Thirty equally spaced contour lines from $p = 1$ to $p = 8$.

265 on the triangular grid. On the other hand, all the schemes of which the dissipative density term does not fulfill Eq.26 are showing carbuncle-free results even on the triangular grid. In particular, the Roe MR scheme, in which $D^{(p)} \neq 0$, is also showing a shock stable result. It is not suggesting that the pressure terms in the numerical mass fluxes are not affecting the shock stabilities. It is more likely that the perturbations introduced
 270 by the pressure term or the grid irregularity are damped by the dissipative density term of rotated upwind schemes, as the similar result of the grid-aligned Roe scheme [22].

6. A pressure-weighted rotation strategy

For the rotated upwind schemes, the previous paragraphs are suggesting that the extra dissipation of the density term in numerical mass fluxes will dump the shock instabilities. Meanwhile, the rotated upwind schemes are showing deteriorated accuracy
 275 in the simulations of viscous flows. Because the monotonicity of the dissipation with rotation angle is shown, it will be possible to find a strategy to improve the performance

of rotated upwind schemes. A straightforward strategy is to control the rotation angle by the shock strength. Here, the rotated Roe scheme is redefined by using the strategy.

280 6.1. Roe WR-M scheme

The key of the proposed strategy is tuning the dissipation by local shock strength, therefore a shock detection method is requested. The hybrid FVS scheme of Drikakis and Tsangaris [10] used the eigenvalues of numerical split fluxes as indicators for the activation of the second-order dissipation terms. Quirk [2] presented a pressure-based switching function for the adaptive application of HLLE scheme [33]. Here, the pressure-weight function of Kim et al [34] is used as a basic indicator of shock strength. The function is

$$f = 1 - \min\left(\frac{p_L}{p_R}, \frac{p_R}{p_L}\right)^3. \quad (31)$$

This function value is gradual changing by the pressure difference at two sides of a interface, and the function has proved to be stable for switching flux functions.

When the numerical flux across a certain cell interface needs to be calculated, as shown in Fig.11, the shock-detective function for the hybridization of fluxes should examine all the adjacent interfaces [22]. Here, the function is defined for selecting the maximum f_k value at the interfaces of both cell i and j :

$$\omega = \max_k(f_k) \quad (32)$$

In regions of smooth flows, f_k of each interface will be in a similar magnitude, and thus the maxima function will not significantly affect calculation results.

285 For simplicity, the left or right pressure in function f is directly using the left or right cell center value, in both first-order and second-order spatial accuracy applications. In the regions of strong shocks, the difference between left and right pressure is large, and thus the function value ω will be approximately equal to 1. In regions of smooth flows, the function value will be very small. Therefore, the function ω will be
290 suitable for indicating the existence of shock waves.

The rotation angle is then defined as

$$\alpha = \frac{\pi}{4} * \omega. \quad (33)$$

Figure 11: Illustration of referenced pressure weight functions, f_k , of the present shock-detective function, ω , for the calculation of an unknown flux, $\Phi_{1/2}$.

Ultimately, the rotation angle is determined by the strength of the local pressure difference. In the vicinity of a strong shock, the angle α will be approximately equal to 45 degree. Conversely, the grid-aligned or "nearly" grid-aligned scheme, in which the α is approximately equal to 0 degree, will be used in the region without strong pressure discontinuity. Therefore, according to the previous analyses, the extra dissipation of the rotated Roe scheme will be introduced only for the calculation of shock waves. Here, the presented rotated Roe scheme is named as Roe WR-M (Weighted Rotation-Multidimensional) scheme for brevity.

6.2. Notes on three-dimensional cases

In three-dimensional cases, the unit direction vector $\mathbf{n}_3$ which obeys conditions $\mathbf{n}_1 \cdot \mathbf{n}_3 = 0$, $\mathbf{n}_2 \cdot \mathbf{n}_3 = 0$ and $C_3 = \mathbf{n}_3 \cdot \mathbf{n}$, needs to be introduced. In the rotated schemes of Ren or Nishikawa, $\mathbf{n}_3$ could be defined by a simple cross product of $\mathbf{n}_1$ and $\mathbf{n}_2$, and thus C_3 is equal to zero. Correspondingly, the $\mathbf{n}_3$ is not directly contributing to the calculation of numerical fluxes.

The newly proposed definition of directions $\mathbf{n}_1$ and $\mathbf{n}_2$ is given by Eq.13. In three-dimensional cases, the $\mathbf{n}_3$ should be defined specifically. Here, the local flow velocity direction is introduced as $\mathbf{n}_V \parallel (\mathbf{V}_L + \mathbf{V}_R)$, at each interface, and then $\mathbf{n}_3$ will be defined to be parallel to $\mathbf{n}_V \times \mathbf{n}$. In other words, the rotation of two directions, $\mathbf{n}_1$ and $\mathbf{n}_2$, will be performed in a plane constructed by the flow velocity direction $\mathbf{n}_V$ and face normal direction $\mathbf{n}$. In fact, the inconsistent normal momentum distribution along shock front, which was suggested to be the source of shock instabilities [35], could be dumped by

the dissipative term that is produced in the rotation plane of each interface. This is because the dissipative term that smear the contact surface could also dump the tangent velocity discontinuity, and then the momentum perturbation could be suppressed. Similar behaviors could be found in two-dimensional cases, in which the velocity direction of each interface is naturally parallel to the rotation plane.

It should be noted that, in a two-dimensional interface or the rotation plane of a three-dimensional interface, there are two choices of rotation direction. However, although the results are not shown here, it is found that the choices are making little difference in the numerical results. For this numerical phenomenon, although a rigorous analysis is not made, the reason is believed to be the general tendency of the dissipation increase which is discussed in subsection 4.2 will not be changed by the choice of rotation direction.

Although the analyses in subsection 4.2 could be extended to three-dimensional by adding $\mathbf{n}_3$ and C_3 into the formulas, it is unnecessary for the cases of which the C_3 is equal to zero. As analysed by Ren [13], the multidimensional effects of shock stability request an adequate selection of upwind-differencing direction, which is closely related to the direction of local flow feature. And thus the dissipation behaviors in the three-dimensional rotation procedure could be complicated. In this paper, most of the discussions and numerical cases concentrate on two-dimensional cases. However, for completeness, a three-dimensional numerical cases is presented in the next subsection.

6.3. Numerical results

By using the proposed rotation strategy, more dissipation will be introduced into flux calculations. Therefore, numerical cases on viscous flow simulations are shown at first, by which the accuracy of the rotated scheme will be clarified. Here, flat plate laminar boundary layer flow and subsonic flow around a cylinder are both calculated. In Fig.12(a), an accurate velocity profile of laminar boundary layer is presented. The separated wake behind the cylinder is shown in Fig.12(b), and the length of the closed wake is presented in Table 1. The length of the calculated closed wake is close to the numerical result of the grid-aligned Roe scheme and the experiment result. These results are produced due to the rotated scheme Roe WR-M is acting as the grid-aligned

(a) Velocity profile of laminar boundary layer (b) Streamline of subsonic flow around cylinder

Figure 12: Viscous flow simulation results of Roe WR-M scheme.

Roe scheme in the boundary layer and wake region, which are showing small pressure-gradient.

The simulation of inviscid hypersonic flow around a cylinder is made by the proposed rotated scheme. As the former work on upwind-differencing schemes [36], in order to investigate the effects of Mach number, numerical simulations of a wide range Mach number are performed (the other conditions are the same as in subsection 5.3). Part of the results are shown in Fig.13. The Roe WR-M scheme is showing carbuncle-free results in all the cases. Whereas, the Roe scheme is failed to produce shock stable results in these cases. This is a evidence that the extra dissipation nearby the shock wave has dumped the shock instability. In these cases, the shock-detective function introduces the extra dissipation based the pressure-difference at each interface, and shows adaptability on the variation of Mach number.

The double-Mach reflection (DMR) problem is simulated for showing the performance on unsteady problem. This problem was studied extensively by Woodward and Colella [37]. Initially, a Mach 10 shock wave is located at $x = 0$, and then the moving shock travels in the x -direction and encounters a wedge that makes an angle 30° with the shock propagation (x -direction). The air ahead of the shock wave has a state $(\rho, u, v, p) = (1.4, 0, 0, 1)$. The computational domain is $[-0.5, 2.5] \times [0, 2.5]$ and a 300×300 quadrilateral grid is used for discretization. The computations use the

Figure 13: Mach contours of inviscid hypersonic flow around a cylinder (Roe WR-M on quadrilateral grid). Thirty equally spaced contour lines from minimum Mach number to maximum Mach number.

explicit Runge-Kutta scheme for temporal solution. The rotated scheme is also compatible with the implicit scheme as in [38]. The CFL is 1 and computations run up to the dimensionless time $t = 0.2$. The second-order finite volume method is used for spatial discretization. The Venkatakrishnan's limiter, of which the parameter K is set
 365 as 1, is used for remaining the monotonicity in the vicinity of shock waves. The results are shown in Fig.14. For the Roe scheme the primary Mach stem is kinked. Whereas, the rotated scheme Roe WR-M is showing shock stability.

As shown in Fig.15, a three-dimensional case is also used to examine the Roe WR-M scheme. The $120 \times 80 \times 25$ grid for the simulation of hypersonic flow around
 370 a cylinder is made by extruding the two-dimensional quadrilateral grid along the z -direction. The other calculation conditions remain the same as the two-dimensional case of which the Mach number is 20. The rotated scheme is showing carbuncle-free result in this case. Whereas, the Roe scheme shows significant carbuncle phenomenon.

Figure 14: The density contours of the double Mach reflection problem. Thirty equally spaced contour lines from $\rho = 4$ to $\rho = 24$.

Figure 15: a) Snapshots of developing 3-D carbuncle of Roe E-Fix. b) A carbuncle-free result of Roe WR-M. Thirty equally spaced Mach contour lines from 0.0 Mach to 20.0 Mach and iso-Mach-number surface of 1.0 Mach.

6.4. Notes on the tunable dissipation

375 These results prove that the dissipation of rotated upwind schemes could be well
tuned by the presented rotation strategy, and shock stability and contact resolved ca-
pability could be acquired at the same time. It should be noted that the application of
tunable dissipation for improving shock stability is not new. The hybrid FVS scheme
of Drikakis and Tsangaris [10] was directly applying a second-order artificial dissipa-
380 tion on the FVS scheme. Besides, the artificial dissipation could also be used on FDS
schemes. On the other hand, the hybrid scheme that combines upwind fluxes [2] was
introducing the tunable dissipation by adaptively applying the dissipative flux function.
This strategy has led to a series of subsequent works. In this paper, comparisons to
other hybrid schemes are not presented due to the depth of the scope. However, the pro-
385 posed rotated scheme shows a different way of exploiting the dissipation mechanism
of rotated schemes.

7. Conclusions

In this work, the shock stability and contact resolving capability of rotated upwind
schemes are investigated by theoretical and numerical investigations. Three typical and
390 commonly used upwind schemes, including Roe scheme, AUSM⁺ scheme, Van Leer
scheme, and their rotated versions are discussed.

Based on the former researches, theoretical analyses are conducted by investigating
the dissipative terms in the numerical mass fluxes of upwind schemes. The dissipative
terms of three grid-aligned upwind schemes are briefly introduced and then the rotated
395 upwind schemes are analysed. In general, the rotation procedure will change the dis-
sipative terms. Most importantly, the dissipative density term, which is critical for the
exact solution of contact discontinuity, will be changed. Therefore, the accuracy of ro-
tated upwind schemes will be deteriorated. On the other hand, the dissipative pressure
term is not equal to zero in both the rotated Roe scheme and grid-aligned Roe scheme.
400 That means the dissipative pressure term will not be essentially changed by the rotation
procedure.

In the numerical cases, it is confirmed that the accuracy of the simulations for viscous flow will be deteriorated by the rotation on the upwind differencing direction. Thereinto, the rotated upwind schemes show inaccurate results in the simulations of flat plate boundary layer flow and subsonic flow around a cylinder. Furthermore, the monotonicity of the dissipation of the rotated schemes with their rotation angle is found in the simulations. Shock stabilities of the rotated schemes are also tested. The rotated schemes show shock stable results on both the quadrilateral grid and triangular grid. A pressure-weighted rotation strategy is then introduced, and showing both shock stability and accurate resolution for contact discontinuity. Different from the former researches that concentrate on a physical meaningful upwind direction, the tuneable dissipation of the presented strategy is determined mainly by the dissipative terms in the numerical mass flux, and could be controlled by the rotation angle of upwind direction. Numerical results prove that the dissipation of the proposed rotation strategy could be effective for suppressing the momentum perturbation which might causes multidimensional shock instabilities.

Further conclusions can be made based on above direct observations. As mentioned in former researches, perturbations could be evolved by the pressure term in numerical mass flux, thus the shock stabilities of upwind schemes are related to the dissipative pressure term. However, the condition $D^{(p)} = 0$ is not sufficient for a scheme to prevent the shock instability from occurring, especially while the simulations are performed on unstructured grid. On the other hand, the perturbations can be effectively dumped by a proper dissipative density term. This is why the rotated upwind schemes are showing intrinsic dissipative property. The intrinsic dissipation, which is essentially introduced by the inaccurate estimation on the velocity of contact discontinuity, will deteriorate the resolution of contact discontinuities and improve the shock stabilities. Therefore, the performance of upwind schemes can be improved by adaptively tuning the dissipation.

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