Bh14 2s?tCMN.BNN03X%7%s%]%8%&%'
E02-5

Upwinded-State-at-the-Face Schemes for Computational Fluid Dynamics

○ Igor' SOKOLOV, Jun-ichi SAKAI, Laboratory of Plasma Astrophysics, Toyama University
Gofuku 3190, Toyama 930-8555, Japan, E-mail: sokolov@ecs.toyama-u.ac.jp
Eugene TIMOFEEV, Kazuyoshi TAKAYAMA, Shock Wave Research Center, IFS, Tohoku University
2-1-1 Katahira, Aoba-ku, Sendai 980-8577, Japan, E-mail: timo@ceres.ifs.tohoku.ac.jp

Recently proposed Artificial Wind concept allows to construct simple and efficient upwind schemes. Here we consider a new class of shock capturing numerical schemes using the Artificial Wind as a building block. These new schemes compute the numerical flux as an exact function of some hydrodynamic state ("Upwind State at the Face" – USF), which may be found using some upwind procedure. The Godunov scheme represents a particular case of the USF schemes. This approach helps to find some new schemes which are rather simple and, on the other hand, ensure high quality results.

1. Introduction

Among the high quality numerical schemes for CFD the Godunov scheme is one of the most popular algorithms [1]. It is based on the exact solution of the Riemann problem (or, in other words, on an exact Riemann Solver) and has an important property not to decrease the entropy. The generalizations of this scheme (Godunov-type schemes) were naturally defined (see [1]) as the schemes using approximate Riemann solvers increasing the entropy.

We choose a new principle to generalize the Godunov scheme and consider the schemes in which, first, the numerical flux is calculated as the exact hydrodynamic flux function $\mathbf{F}(\mathbf{U}_{\mathrm{USF}})$ of some Upwinded State at the Face (USF) and, second, this hydrodynamic state is constructed using some upwinding procedure. One particular case of such procedures coincides with the exact solution of the Riemann problem. All other USF schemes can hardly be interpreted as being based upon some approximate solution of the Riemann problem because such solution would be a manifold function of a spatial coordinate.

As a building block for constructing USF schemes we also use the recently proposed Artificial Wind (AW) schemes [2-3]. Although the AW schemes have been already published in detail we give below a brief review. Then we elaborate the USF concept and show how the Differential AW scheme can be coupled with an USF scheme.

2. Artificial Wind scheme

We paid attention to and used the following fact: the "technological complexity" of the upwinding problem is not Galilean invariant while the hydrodynamic equations are certainly Galilean invariant. That is why it is always possible to choose a frame of reference which moves with a velocity D with respect to the original frame of reference in such a way that all the flow under consideration becomes supersonic in the new frame. An additional velocity $-D$ is added to the velocity of the flow in the moving frame of reference making the flow to be supersonic. We refer to this velocity as an Artificial Wind (AW) velocity in order to emphasize that its value is a matter of our choice and that it is introduced to facilitate upwinding. The problem of upwinding becomes trivial in the moving frame of reference because in supersonic flows all perturbations propagate along one definite direction depending upon the direction of the AW velocity. The procedure for "remapping" of numerical solution from the moving frame of reference to the original one may be arranged by several ways [2-3].

Instead of using a moving frame of reference, one may consider a spatial-temporal invariance of an arbitrary hyperbolic system $\partial\mathbf{U}/\partial t + \partial\mathbf{F}/\partial x = 0$, where $\mathbf{U}$ is the vector of conserved variables, $\mathbf{F}$ is the vector of their fluxes, t – time and x – a spatial coordinate. The equations are obviously invariant with respect to the transformation of time and space $t' = t$, $x' = x - Dt$ as long as the flux and the Jacobian matrix $\mathbf{A} = \partial\mathbf{F}/\partial\mathbf{U}$ are also transformed as follows:

$$\mathbf{F}' = \mathbf{F} - D\mathbf{U}, \ \ \mathbf{A}' = \mathbf{A} - D\mathbf{E}. \tag{1}$$

Thus, all perturbations may be converted into those moving in the positive direction of x-axis (all eigenvalues of the Jacobian matrix become positive) or into those moving in the negative direction of x-axis (if all eigenvalues of the Jacobian matrix become negative) using solely the transformation (1) (the AW transformation).

This idea may be applied for constructing the first order numerical flux $\mathbf{F}_{i-1/2}$ via a face between two control volumes considering one-dimensional Euler equations at equally spaced (Δx) grid as the simplest example. The values of the conserved variables, averaged over two adjacent control volumes are $\mathbf{U}_{i-1}$ and $\mathbf{U}_i$. In order to decrease the numerical dissipation we should not limit AW velocities by the values based on the *averaged* conserved variables . We propose to assign them separately for each of the *intermediate states between* $\mathbf{U}_{i-1}$ and $\mathbf{U}_i$ which may be obtained using linear interpolation with the weight coefficient ξ ($0 \le \xi \le 1$): $\overline{\mathbf{U}}(\xi, \mathbf{U}_{i-1}, \mathbf{U}_i) = (1-\xi)\cdot\mathbf{U}_{i-1} + \xi\cdot\mathbf{U}_i$. When integrating the Jacobian matrix $\mathbf{A}$ over the intermediate states we apply the AW transformation for the Jacobian under integration and obtain:

$$\mathbf{F}_i - \mathbf{F}_{i-1} = \int_0^1 (\mathbf{A}(\overline{\mathbf{U}}(\xi)) - D(\xi)\mathbf{E})\mathrm{d}\xi \times (\mathbf{U}_i - \mathbf{U}_{i-1}) \tag{2}$$

as long as the following condition is satisfied: $\int_0^1 D(\xi)\mathrm{d}\xi = 0$. Now we choose the velocities of the *Differential* AW in the following way: $D(\xi) = D^R(\xi) \ge \max(0, v(\xi) + c(\xi))$, for $\xi \in (0, \xi^*)$ and $D(\xi) = D^L(\xi) \le \min(0, v(\xi) - c(\xi))$ for $\xi \in (\xi^*, 1)$. As a result the integration in Eq.(2) between the limits 0 to ξ^* becomes a sum of perturbations propagating to the left, because $\mathbf{A}(\overline{\mathbf{U}}(\xi)) - D(\xi)\mathbf{E}$ has only negative eigenvalues. Then for the remaining part of the interval $\xi \in (\xi^*, 1)$ the integral becomes a sum of perturbations propagating to the right. The flux difference $\mathbf{F}(\mathbf{U}_i) - \mathbf{F}(\mathbf{U}_{i-1})$ is thus splitted and the problem of upwinding is solved. Constructing the numerical first order upwind flux in a usual manner and calculating the integral in Eq.(2) one can get a very simple flux formula:

$$\mathbf{F}_{i-1/2} = \mathbf{F}(\xi^*\mathbf{U}_i + (1-\xi^*)\mathbf{U}_{i-1}) + d\cdot(\mathbf{U}_{i-1} - \mathbf{U}_i) \quad (3)$$

where the diffusion coefficient is $d = \int_0^{\xi^*} D^R(\xi)\mathrm{d}\xi = -\int_{\xi^*}^1 D^L(\xi)\mathrm{d}\xi$. The velocities $D^R(\xi)$ and $D^L(\xi)$ may be taken to be equal to their limiting values (see inequalities above). Iteration procedure for easily finding the values of ξ^* and d was described in [3].

3. Upwinded State at the Face

To investigate the relationship between the Godunov and Differential AW schemes we propose to consider a new class of upwind schemes with the numerical flux being the *exact* flux function $\mathbf{F}(\mathbf{U}_{USF})$ of some *Upwinded State at the Face* (USF) which is constructed using some appropriate upwinding procedure.

For the Godunov scheme the numerical flux may be also written as the flux function of an USF:

$$\mathbf{F}_{i-1/2} = \mathbf{F}(\mathbf{U}_{RS}(\mathbf{0}, \mathbf{U}_{i-1}, \mathbf{U}_i)) \quad (4)$$

where $\mathbf{U}_{RS}(x/t, \mathbf{U}_L, \mathbf{U}_R)$ is the solution of the Riemann problem for the step-like initial condition ($t = 0$): $\mathbf{U}(0,x) = \mathbf{U}_L$, $x < 0$; $\mathbf{U}(0,x) = \mathbf{U}_R$, $x > 0$. The upwind property of the USF $\mathbf{U}_{RS}(0, \mathbf{U}_{i-1}, \mathbf{U}_i)$ may be illustrated by the fact that all physical perturbations in the exact RS have the velocities of propagation which are directed *out of the face*. To the contrary, the property of the numerical flux to be an exact flux function of some USF is not pertinent to Godunov-type schemes with approximate Riemann solvers [1,4,5].

Now let us discuss general features of the numerical schemes, for which the numerical flux is an exact flux function of an USF:

$$\mathbf{F}_{i-1/2} = \mathbf{F}(\mathbf{U}_{USF}(\mathbf{U}_{i-1}, \mathbf{U}_i)). \quad (5)$$

The USF is proposed to be constructed according to the following rules. The flux difference $\mathbf{F}_{i-1/2} - \mathbf{F}_{i-1}$ is assumed to be representable as a (finite or infinite) sum of physical perturbations propagating to the left:

$$\mathbf{F}(\mathbf{U}_{USF}) - \mathbf{F}(\mathbf{U}_{i-1}) = \sum_{j=1}^{J}(\mathbf{F}(\mathbf{U}^{(j+1)}) - \mathbf{F}(\mathbf{U}^{(j)})), \quad (6)$$

$$\mathbf{U}^{(1)} = \mathbf{U}_{i-1},\ \mathbf{U}^{(J+1)} = \mathbf{U}_{USF}.$$

In the same way, the flux difference $\mathbf{F}(\mathbf{U}_i) - \mathbf{F}(\mathbf{U}_{USF})$ should be represented as the sum of physical perturbations propagating to the right. For a linear hyperbolic system of equations ($\mathbf{F} = \mathbf{AU}$, $\mathbf{A}$ being the constant matrix) the flux differences $\mathbf{F}(\mathbf{U}^{(j+1)}) - \mathbf{F}(\mathbf{U}^{(j)})$ are the amplitudes of the linear eigenmodes propagating to the left, the states $\mathbf{U}^{(j)}$ being the constant states between the fronts of eigenwaves. The numerical flux $\mathbf{F}(\mathbf{U}_{USF}(\mathbf{U}_{i-1}, \mathbf{U}_i))$ coincides with that of the upwind scheme for the linear system.

For a non-linear system the velocity of perturbations may be introduced in the following way. First, for infinitesimal perturbations, i.e. when the difference $\mathbf{F}(\mathbf{U}^{(j+1)}) - \mathbf{F}(\mathbf{U}^{(j)})$ in the Eq.(6) is infinitely small, it may be represented as $\mathbf{F}(\mathbf{U}^{(j+1)}) - \mathbf{F}(\mathbf{U}^{(j)}) \approx \mathbf{A}(\mathbf{U}^{(j)})d\mathbf{U}^{(j)}$, $d\mathbf{U}^{(j)} = \mathbf{U}^{(j+1)} - \mathbf{U}^{(j)}$, where $\mathbf{A} = \partial\mathbf{F}/\partial\mathbf{U}$ is the Jacobian of a non-linear system. The flux difference may be associated with the physical perturbation propagating to the left if $d\mathbf{U}^{(j)}$ is an arbitrary infinitesimal linear combination of only those eigenvectors (normal modes) of the Jacobian $\mathbf{A}(\mathbf{U}^{(j)})$ which correspond to the *non-positive* eigenvalues (velocities of normal modes). With this requirement and with an obvious transition from finite sums to integration we find that the sums in the Eqs.(6) may involve an integral over a path in a space of the conserved variables $\int \mathbf{A}(\mathbf{U})d\mathbf{U}$ with the following restriction on the integration path: the vector $d\mathbf{U}$ is a linear combination of the eigenvectors of the Jacobian $\mathbf{A}(\mathbf{U})$ corresponding to non-positive eigenvalues (the Left-Perturbation path or LP-path). If the vector $d\mathbf{U}$ is a linear combination of the eigenvectors of the Jacobian $\mathbf{A}(\mathbf{U})$ corresponding to non-negative eigenvalues the path is referred to as the RP-path (the Right-Perturbation path), respectively.

The velocity of a finite amplitude perturbation may be correctly defined if and only if it is a ***physical discontinuity*** satisfying the Rankine-Hugoniot relation $\mathbf{F}(\mathbf{U}^{(j+1)}) - \mathbf{F}(\mathbf{U}^{(j)}) = \Lambda^{(j)}(\mathbf{U}^{(j+1)} - \mathbf{U}^{(j)})$.

So, finally the Eq.(6) may be written as

$$\mathbf{F}(\mathbf{U}_{USF}) - \mathbf{F}(\mathbf{U}_{i-1}) = \int_{\mathbf{U}_{i-1}}^{\mathbf{U}_{USF}} \mathbf{A}(\mathbf{U})d\mathbf{U} \quad (7)$$

where the integration path is piecewise continuous. All the continuous parts should be LP-paths, and integration there is treated in a usual sense. Discontinious parts in the integration path are acceptable only if the Rankine-Hugoniot relations are fulfilled across such discontinuities, the value of Λ being non-positive and the integral at this jump is treated in a sense of the following substitution: $d\mathbf{U} \to \mathbf{U}^{(j+1)} - \mathbf{U}^{(j)})$, $\mathbf{A} \to \Lambda\mathbf{E}$, where $\mathbf{E}$ is the unit matrix.

On the other hand, the difference $\mathbf{F}(\mathbf{U}_i) - \mathbf{F}(\mathbf{U}_{USF}(\mathbf{U}_{i-1}, \mathbf{U}_i))$ may be represented as follows:

$$\mathbf{F}(\mathbf{U}_i) - \mathbf{F}(\mathbf{U}_{USF}) = \int_{\mathbf{U}_{USF}}^{\mathbf{U}_{i+1}} \mathbf{A}(\mathbf{U})d\mathbf{U} \quad (8)$$

with piece-wise continuous integration path with all continuous pieces being RP-paths while each discontinuitity satisfies the Rankine-Hugoniot relations with non-negative propagation velocities.

Let us introduce an additional requirement that all continuous parts of the LP- and RP-paths are simple (Riemann) waves. These exact non-linear solutions are usually rather simple and the propagation velocity for them may be readily computed. Now one can ***define*** the USF $\mathbf{U}_{USF}(\mathbf{U}_{i-1}, \mathbf{U}_i)$ as such set of the conserved variables that the integration paths in Eqs.(7,8) do exist and satisfy the requirements specified above. Let us emphasize that no integration is actually to be performed. It is sufficient to connect the left and right states $\mathbf{U}_{i-1}$, $\mathbf{U}_i$ by a piece-wise continuous path following some procedure, find the point $\mathbf{U}_{USF}(\mathbf{U}_{i-1}, \mathbf{U}_i)$ (which separates the perturbations propagating to the left and to the right) at this path, and then compute the flux Eq.(5).

For example, in the Godunov scheme the (unique) path is specified by the only additional requirement: the velocity of propagation λ insreases monotonically along the path from $\mathbf{U}_{i-1}$ to $\mathbf{U}_i$. As a consequence, the conserved variables may be represented as the functions of λ. This dependence is in fact the Riemann Solver (RS).

Without the requirement for the propagation velocity to be monotone, the integration path is not unique. For a perfect gas with a constant polytropic index another integration path may be easily constructed, consisting of the right simple wave passing through the state $\mathbf{U}_i$, the left simple wave passing through the state $\mathbf{U}_{i-1}$ as well as the contact discontinuity connecting some pair of states at these simple waves. Such integration path is introduced in the Osher scheme [5][1]. The computation of USF is easy, no iteration procedure is required. Due to non-monotone character of the propagation velocity in simple compression waves the path can not always be splitted into LP-path and RP-path: this is impossible if the compression simple wave(s) involves a sonic point. This obstacle can be readily overcome by means of substituting the compression wave with a sonic point by a combination of a stationary shock wave followed by a simple compression wave.

The procedure to construct the path is straightforward. For a right simple wave passing through the state $\mathbf{U}_i$ the dependence of pressure from velocity is found. The analogous dependence is also found for the left simple wave passing through the state $\mathbf{U}_{i-1}$. The dependencies obtained are matched using the condition for pressure p_c and velocity v_c to be continuous at the contact discontinuity. For a perfect gas with a constant polytropic index the equation for v_c is linear and may be easily solved. If any of the simple waves appears to be a compression wave involving a sonic point (rather rare situation), a standing shock wave(s) is introduced and the path construction is repeated. Procedure for finding USF is easy and, for a gas, reduces to solving only simple linear equations even for strongly non-linear waves.

The test results and theoretical considerations for the latter USF scheme show that for CFL numbers close to 1 the positivity of the entropy production is ensured only if the simple compression waves are not too strong, namely:

$$v_{i-1} - c_{i-1} < v_c < v_i + c_i \tag{9}$$

One can readily see that the condition Eq.(9) may be invalid if the amplitude of the simple compression wave is large enough. We think that this condition is of rather general nature and the rejection of the monotone velocity principle (as in the RS) and the introduction of simple compression waves may only be considered at the cost of the requirement that the amplitudes of these compression waves should be restricted by some finite value.

4. USF+AW schemes

Now we show how to incorporate AW into an USF scheme. The simplest way to do it is to assign *any* state $\mathbf{U}^{(L)}_{USF}$ of LP-path as the left state for differential AW scheme, and *any* state of RP-path as the right state for differential AW scheme. Combining the Eqs.(2,7,8) one can get a general formula as follows:

$$\mathbf{F}(\mathbf{U}_i) - \mathbf{F}(\mathbf{U}_{i-1}) = \int_{\mathbf{U}_{i-1}}^{\mathbf{U}^{(L)}_{USF}} \mathbf{A}(\mathbf{U})d\mathbf{U} +$$

$$+\int_0^1 (\mathbf{A}(\overline{\mathbf{U}}(\xi)) - D(\xi)\mathbf{E})d\xi(\mathbf{U}^{(R)}_{USF} - \mathbf{U}^{(L)}_{USF}) + \tag{10}$$

$$+\int_{\mathbf{U}^{(R)}_{USF}}^{\mathbf{U}_{i+1}} \mathbf{A}(\mathbf{U})d\mathbf{U}$$

that is the upwinding is ensured by a proper choice of an integration path for the first and last integrals and by the introduction of Artificial Wind for the central one. of it

[1] In fact, the reverse order of simple waves was used in the original Osher-Chakravarthy scheme but the way described here is also mentioned in [5].

Finally, the numerical flux is as follows:

$$\mathbf{F}_{i-1/2} = \mathbf{F}(\xi^*\mathbf{U}^{(R)}_{USF} + (1-\xi^*)\mathbf{U}^{(L)}_{USF}) + \tag{11}$$

$$+d \cdot (\mathbf{U}^{(L)}_{USF} - \mathbf{U}^{(R)}_{USF})$$

In a particular case of $\mathbf{U}^{(R)}_{USF} = U_i$ and $\mathbf{U}^{(L)}_{USF} = U_{i-1}$ we return to the Diffrential AW scheme, in the opposite case $\mathbf{U}^{(R)}_{USF} = \mathbf{U}^{(L)}_{USF} = \mathbf{U}_{USF}$ - to an USF scheme. Both AW and USF schemes get some advantage out of their combination. Confronting to the Diffrential AW scheme, the numerical dissipation in Eq.(11) may be considerably lower as long as the states $\mathbf{U}^{(R)}_{USF}$ and $\mathbf{U}^{(L)}_{USF}$ are closer to each other as compared to U_i and U_{i-1}. As compared to an USF scheme, the use of the Eq.(11) allows to ensure *any* given restriction for an amplitudes of the simple waves, e.g. one can use a simple (for example, linear) solver for smooth numerical solutions as well as reasonable numerical dissipation for large gradients which is a little bit lower as compared to the pure AW scheme.

As a practical example for a test simulation we have employed an USF scheme with non-linear simple waves (both compression and rarefaction ones) for a gas with a constant polytropic index ($\gamma = 7/5$), in the way as discussed above. The AW is introduced only in case the condition Eq.(9) is not hold between the states $\mathbf{U}^{(L)}_{USF}$ and $\mathbf{U}^{(R)}_{USF}$, each of them satisfying the condition Eq.(9). To extend the scheme up to the second order of accuracy, we insert the first order solver into the Rodionov scheme [6], using the interpolation over primitive variables and β - limiter [5] with $\beta = 1.6$.

The simulation results for the Woodward-Collela test problem [7] is presented in Fig.1 with the results for the Rodionov scheme (a second order extension of the Godunov scheme with an exact Riemann solver) given for a comparison. CFL number is equal to 0.8 for both simulations. It is clearly seen that the results are at least of the same quality as that of the Rodionov scheme involving an exact Riemann solver.

5. Conclusion

The recently proposed AW schemes give good numerical results as applied for hydrodynamic problem with complex physics. It is closely related to another new class of numerical schemes, namely, the USF schemes discussed in detail in the present paper.

The high quality test results show that the coupling of the AW scheme and the newly proposed USF approach seems to be very promising. Using such a coupling we may have an opportunity to take advantage of it, for instance, giving "priority" to the USF or AW parts of the combined scheme depending upon local characteristics of the solution (smooth solution or a discontinuity).

References

1. Harten A., Lax P.A., van Leer B. "On upstream differencing and Godunov-type schemes for hyperbolic conservation laws", 1983, SIAM Review, V.25, p.35.
2. Sokolov IV, Timofeev EV, Sakai J, Takayama K, "On shock-capturing schemes using artificial wind", *Shock Waves Journal*, 1999, V.9, p.423.
3. Sokolov IV, Timofeev EV, Sakai J, Takayama K, " Development and applications of artificial wind schemes for hydrodynamics, MHD and relativistic hydrodynamics", Proc of the 13th Japanese CFD Conf, Tokyo, Chuo Univ, Dec. 1999
4. Toro E. Riemann Solvers. Springer, 1997.
5. Hirsch C. Numerical computation of internal and external flows, V.2, Wiley, 1990.

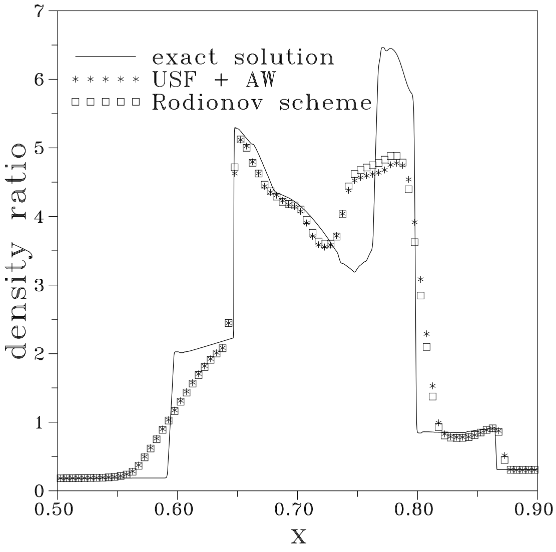

Fig. 1: The comparison of the numerical results for Woodward - Collela test: the solid line shows "theoretical" distribution; squares present the numerical results for the Rodionov scheme with the exact RS; star symbols give the test results for USF scheme coupled with the Differential AW scheme.

6. Rodionov A.V. "Improvement of the approximation order in the Godunov scheme", Zh.Vychisl.Mat.Mat.Fiz, 1987, v.27, pp.1853-1860 (in Russian)
7. Woodward P.R., Collela P., "The numerical simulation of two-dimensional flows with strong shocks", Journal of Comp.Phys., 1984, v.54, pp.115-173