Journal of Computational Physics: X 8 (2020) 100077

Contents lists available at ScienceDirect

Journal of Computational Physics: X

www.elsevier.com/locate/jcpx

On an inconsistency of the arithmetic-average signal speed estimate for HLL-type Riemann solvers

Nico Fleischmann *, Stefan Adami, Nikolaus A. Adams

Technical University of Munich, Department of Mechanical Engineering, Chair of Aerodynamics and Fluid Mechanics, Boltzmannstraße 15, 85748 Garching, Germany

A R T I C L E I N F O

Article history:
Received 21 April 2020
Received in revised form 11 September 2020
Accepted 25 September 2020
Available online 30 September 2020

Keywords:
Approximate Riemann solver
HLL
HLLC
Signal speed estimates
Low-dissipation scheme

A B S T R A C T

In this short note, we highlight the sensitivity of the HLL-type Riemann solver with respect to the choice of signal speed estimates and demonstrate a major deficiency of the arithmetic-average estimate. The investigation of two essential Riemann problems and a classical bow shock simulation reveals that inherent inconsistencies of the arithmetic-average estimate may lead to unexpected behavior and erroneous results.

1. Introduction

The development of computationally cheap but nevertheless stable and accurate approximations of the Riemann problem is crucial for the success of Godunov-type methods [1] in computational fluid dynamics. In combination with high-order discretizations, such as WENO schemes [2], these approximate-flux solvers have become popular nowadays for the simulation of complex multi-scale flow problems, e.g. shock interactions with phase interfaces or turbulent flows [3]. In particular, Roe and HLL-type Riemann solvers are applied in various state-of-the-art compressible flow solvers due to their favorable low numerical dissipation [4–6]. Common for such solvers is the need for proper estimations of the wave signal speeds. An overview of the topic can be found in [3]. In this short note, we highlight the sensitivity of the HLL-type Riemann solver with respect to the choice of signal speed estimates and demonstrate a major deficiency of the arithmetic-average estimate, which has become increasingly popular in recent publications [7–10].

In their fundamental work, Harten, Lax and van Leer [5] proposed design principles for simple but nevertheless robust approximate Riemann solvers where left and right states are linked through one or two intermediate states separated by waves. They did not propose actual estimates of the essential signal speeds for their approximations. They stated, however, that the estimates for the left- and right-going wave speed have to be lower, respectively upper bounds of the physical wave speeds. The popular HLL and HLLC Riemann approximations result from the combination of these design principles with suitable signal speed estimates as proposed by different authors [11,12,6,13,14].

Both Davis [11] and Einfeldt [12] simultaneously developed signal speed estimates for the HLL approximation. Besides the simple but rarely applied estimates $S_L = u_L - c_L$ and $S_R = u_R + c_R$, Davis also proposed

* Corresponding author.
E-mail addresses: nico.fleischmann@tum.de (N. Fleischmann), stefan.adami@tum.de (S. Adami), nikolaus.adams@tum.de (N.A. Adams).

https://doi.org/10.1016/j.jcpx.2020.100077

$$S_L^{Davis} = \min(u_L - c_L, u_R - c_R), \qquad S_R^{Davis} = \max(u_L + c_L, u_R + c_R) \tag{1}$$

for the minimum signal speed S_L and the maximum signal speed S_R with direct application of the left and right velocity u and speed of sound c. Instead, Einfeldt defines the generalized formulation

$$\hat{c}^2 = \frac{{c_L}^2 \cdot \sqrt{\rho_L} + c_R^2 \cdot \sqrt{\rho_R}}{\sqrt{\rho_L} + \sqrt{\rho_R}} + \frac{1}{2} \frac{\sqrt{\rho_L}\sqrt{\rho_R}}{\left(\sqrt{\rho_L} + \sqrt{\rho_R}\right)^2} \left(u_R - u_L\right)^2 , \tag{2}$$

and the Roe average

$$\hat{u} = \frac{u_L \cdot \sqrt{\rho_L} + u_R \cdot \sqrt{\rho_R}}{\sqrt{\rho_L} + \sqrt{\rho_R}} \tag{3}$$

to determine the final signal speed estimates $S_L = \hat{u} - \hat{c}$ and $S_R = \hat{u} + \hat{c}$ as proposed in [12]. A blend of Davis' approach and Einfeldt estimates delivers slightly improved estimates given by

$$S_L^{Einfeldt} = \min(u_L - c_L, \hat{u} - \hat{c}), \qquad S_R^{Einfeldt} = \max(u_R + c_R, \hat{u} + \hat{c}) \tag{4}$$

which will be denoted 'Einfeldt estimates' for simplicity in the remainder of the paper. Batten et al. [13] proposed similar estimates to Eq. (4) with the only difference being that $\hat{c}$ is determined by the original Roe average instead of the generalized formulation of Einfeldt (2). The contact wave was reconstructed by Toro et al. [6] resulting in the HLLC approximate Riemann solver that covers all physical waves governed by the Euler equations. Moreover, the authors [6] suggested to determine the signal speeds from the constant intermediate pressure p^* instead of calculating them directly. p^* is approximated under the assumption that both nonlinear waves are rarefaction waves. Afterwards, the exact wave relations are applied to determine the signal speed estimates. Finally, Batten et al. [13] proposed an estimate for the velocity of the contact speed in the form of

$$S_* = \frac{p_R - p_L + \rho_L u_L \left(S_L - u_L\right) - \rho_R u_R \left(S_R - u_R\right)}{\rho_L \left(S_L - u_L\right) - \rho_R \left(S_R - u_R\right)}, \tag{5}$$

which follows directly from the acoustic wave speed estimates S_L and S_R, and left and right primitive states. Guermond and Popov [14] were the first to develop signal speed estimates that fulfill the essential boundedness criterion of Harten et al. [5]. They proposed both a direct and a more accurate iterative method to determine bounds for the physical wave speeds. Recently, Toro et al. [15] performed a detailed investigation on the boundedness of various signal speed estimates, where they showed that most established estimates do not bound the physical wave speeds in general. Furthermore, they provided new bound estimates for the fastest wave speeds. In recent publications [7–10], the accurate but computationally expensive Einfeldt signal speed estimate is more and more replaced by the simple arithmetic-average estimate with $\hat{u} = \frac{1}{2}\left(u_L + u_R\right)$ and $\hat{c} = \frac{1}{2}\left(c_L + c_R\right)$. This selection is reported to deliver results that are close to the ones obtained with the original Einfeldt estimate for a broad range of cases. However, the reasoning is highly empirical for strong shocks since a theoretical foundation is only given for sufficiently weak shocks, as remarked by Einfeldt [12]. Indeed, it can be easily shown that the arithmetic-average signal speed estimate contradicts to fundamental assumptions of the underlying Riemann approximation. In the following section, this will be demonstrated in detail for a simple moving shock wave and a steady shock wave. The application of the arithmetic average is particularly problematic for bow shock simulations as shown in detail in the third section. Additionally, a replacement of the original "if" statements by sign functions within the HLLC formulation is discussed. The latter implementation might (almost) completely hide the misbehavior of the arithmetic average.

2. Discussion of signal speed estimates for simple Rankine-Hugoniot shock conditions

First, the described signal speed estimates connected to the HLLC approximation are evaluated for a simple moving shock wave. This special case frequently appears in practical simulations, e.g. after initialization. In this example, we use a fixed pre-shock state with the primitive variables $\rho_R = 1.0$, $v_R = 0$ and $p_R = 1.0$. The left state of the shock is varied along the Hugoniot locus. In Fig. 1, the resulting left (dashed) and right (solid) nonlinear signal speed estimates, and the estimate for the contact velocity (dotted) using Eq. (5) are plotted together with the exact shock speed (bold) for moderate and high Mach numbers ranging from 1.01 to 4 and 1.01 to 20, respectively.

In the following, we analyze the resulting HLLC flux given by Toro et al. [6] in the form

$$\mathbf{F}^{HLLC} = \begin{cases} \mathbf{F}_L & \text{if } S_L \geq 0, \\ \mathbf{F}_{*L} = \mathbf{F}_L + S_L \cdot \left(\mathbf{U}_{*L} - \mathbf{U}_L\right) & \text{if } S_L < 0 \cap S_* \geq 0, \\ \mathbf{F}_{*R} = \mathbf{F}_R + S_R \cdot \left(\mathbf{U}_{*R} - \mathbf{U}_R\right) & \text{if } S_R > 0 \cap S_* \leq 0, \\ \mathbf{F}_R & \text{if } S_R \leq 0, \end{cases} \tag{6}$$

for the different signal speed estimates.

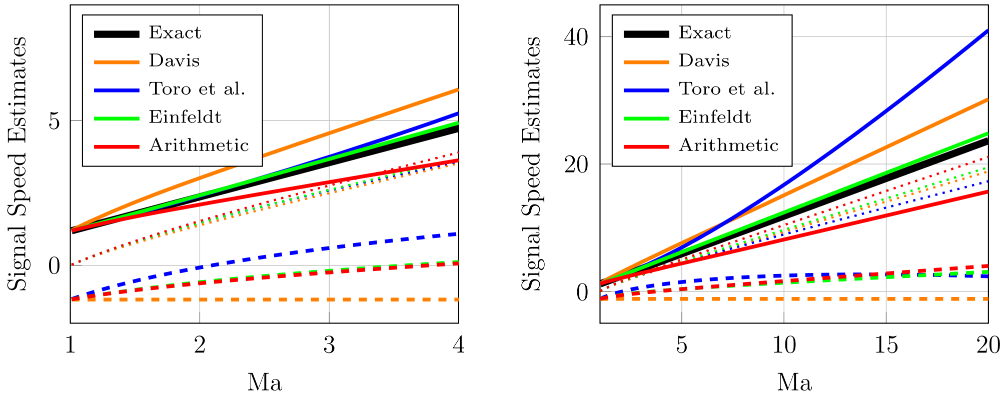

Fig. 1. Signal speed estimates for the HLL(C) approximation evaluated for a simple right-traveling shock wave for different Mach numbers (solid: right; dotted: contact; dashed: left).

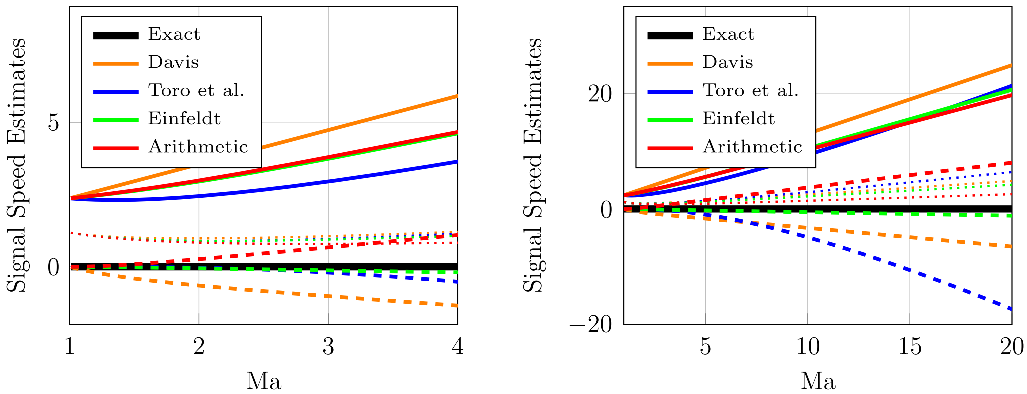

Fig. 2. Signal speed estimates for the HLL(C) approximation evaluated for a simple steady shock wave for different Mach numbers (solid: right; dotted: contact; dashed: left).

A supersonic condition with all signal speeds above zero is predicted for Mach numbers larger than ∼2.1 for the Toro estimate [6], ∼3.5 for the Einfeldt estimate (Eq. (4)-(2)), ∼3.6 for the arithmetic-average estimate and never for the Davis estimate (Eq. (1)). Below these values, the HLLC flux (6) is always given by $\mathbf{F}_{*L}$ since $S_* > 0$ holds true for all Mach numbers and all considered signal speed estimates. Note that $S_L^{Arithmetic}$ and $S_L^{Einfeldt}$ yield nearly identical results.

Although S_R does not directly affect the final flux estimation in this particular case, it is nevertheless interesting to study the differences among the described types of estimates. For moderate Mach numbers, the estimate of Davis considerably overestimates the physical wave speeds, whereas both the estimate of Einfeldt and Toro are only slightly larger. For $Ma > 6.7$, the estimate of Toro predicts the largest right-travelling wave speed, while the estimate of Einfeldt still is close to the physical value. In contrast, the arithmetic-average estimate for S_R systematically underestimates the physical wave speed, and therefore it violates the boundedness criterion of Harten et al. [5]. Moreover, the incorrect nonlinear signal speed estimates lead to an incorrect approximation of the contact velocity. In consequence, S_R even falls below the estimate for the contact velocity for $Ma > 3.3$, which is in contradiction to the fundamental assumption $S_L < S_* < S_R$ [11,12]. However, due to the construction of HLLC this flaw does not affect the resulting flux for simple moving waves. Note, that for $S_L < 0$ the left flux $\mathbf{F}_L$ is used, and for $S_L > 0$ the intermediate flux $\mathbf{F}_{*L}$ is used as $S_* > 0$ for any estimate. Since most practical scenarios consist of such simple moving waves, where the contact wave direction and the flow direction are identical, it can be explained why results obtained with the arithmetic average are often similar to ones obtained with the Einfeldt estimate despite the poor estimate $S_R^{Arithmetic}$. However, in the following we show that is cannot be relied upon.

The same procedure is applied to a steady shock problem with the fixed pre-shock conditions $\rho_L = 1.0$, $u_L = \sqrt{\gamma} \cdot Ma$ and $p_L = 1.0$. Post-shock states are obtained from the Rankine-Hugoniot jump condition for varying Mach numbers. The resulting signal speed estimates are shown in Fig. 2.

A similar qualitative behavior with switched left and right states as compared to the previous case can be observed. Arithmetic-average and Einfeldt estimates for S_R are almost identical. However, as S_* is still strictly positive, now the deviations in S_L directly affect the approximate flux. Again, the physical shock speed is not captured by the arithmetic-average estimate, and $S_L < S_* < S_R$ is violated. Moreover, this estimate leads to a pure supersonic flux selection independently of the Mach number, whereas all other estimates predict a subsonic case. The Einfeldt estimate again is close to the physical wave speed.

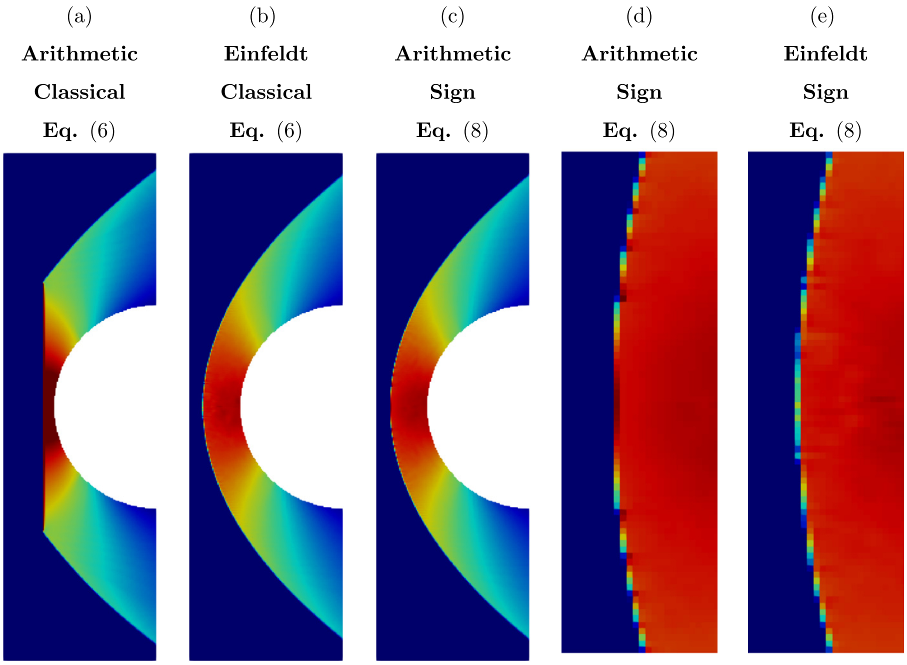

Fig. 3. Supersonic flow around cylinder for different HLLC flux formulations: color pressure map (blue= 1.0 to red= 550) at $t = 0.05$ resolved with 160 cells per diameter.

3. Effect on bow shock calculations

After the discussion of the specific Riemann problems, the adverse effect of the arithmetic-average estimate is now demonstrated for a classical test case, the supersonic flow around a cylinder. The setup and numerical scheme is chosen identical to [16] with a free-stream Mach number of 20. A classical fifth-order WENO scheme [2] has been applied combined with a third-order, explicit, strong stability-preserving time integration [17] using a CFL number of 0.4. The maximum time step is determined by

$$\Delta t = C_{CFL} \cdot \left[\max_{i,k} \left(\frac{|u_{i,k}| + c_{i,k}}{\Delta x} \right) + \max_{i,k} \left(\frac{|v_{i,k}| + c_{i,k}}{\Delta y} \right) \right]^{-1} \tag{7}$$

with u, v being the velocity components, c being the speed of sound and Δx, Δy being the cell dimensions. The simulation has been performed up to a final time of $t = 0.5$, where a fully developed bow shock is observed. The resulting pressure field is shown in Fig. 3(a) and Fig. 3(b) for the HLLC flux with both the arithmetic-average and the Einfeldt estimate. The application of the former leads to a blocking behavior during the built-up process of the bow shock combined with a massive overshoot in pressure and density in the cells along the shock. A similar behavior including the blocking at the bow shock front can be observed when the HLL flux is combined with arithmetic-average estimates (not shown here). The application of the Einfeldt estimate delivers results as described in literature with minor disturbances behind the shock front [16].

A compact formulation of the HLLC flux (6) using the sign function is given e.g. in [18] and reads

$$\begin{aligned} \mathbf{F}^{HLLC} = & \frac{1 + sign(S_*)}{2} \left[\mathbf{F}_L + S^- \left(\mathbf{U}_{*L} - \mathbf{U}_L \right) \right] + \\ & \frac{1 - sign(S_*)}{2} \left[\mathbf{F}_R + S^+ \left(\mathbf{U}_{*R} - \mathbf{U}_R \right) \right], \end{aligned} \tag{8}$$

with $S^- = \min(S_L, 0)$ and $S^+ = \max(S_R, 0)$.

Interestingly, the failure of the arithmetic-average estimate is almost completely hidden when the sign formulation is applied, see Fig. 3(c), where the arithmetic-average estimate was used in combination with the compact formulation (8). This can be explained by a subtle change in the sequence of algorithmic decisions. The classical formulation first evaluates $S_L > 0$ and immediately chooses the supersonic case if this holds true independently of S^*, whereas the sign formulation first evaluates S^*. If $S_L < S_* < S_R$ is valid, this change in the sequence of decisions will not lead to a different result. However, during the built-up process the contact-wave speed for the arithmetic-average estimate is negative, which is correct since the forming bow shock travels upstream towards the steady-state position, while the arithmetic-average estimate for

S_L is positive. In this case, the sign formulation nevertheless detects the correct right part, and happens to ignore the supersonic nonlinear arithmetic-average estimate. The classical formulation reproduces the incorrect supersonic case. A detailed investigation reveals that there are still minor overshoots in density and pressure at the tip of the bow shock also for the sign formulation as shown in Fig. 3(d). When the Einfeldt estimate is applied, the results for both flux formulations are always identical and no overshoot can be observed, see Fig. 3(e).

This example demonstrates that the described shortcomings of the arithmetic-average estimate can lead to unexpected consequences and wrong results that can be efficiently avoided by the application of mathematically consistent estimates.

4. Conclusion

We have shown in detail that the arithmetic-average estimate may deliver comparable results as the Einfeldt estimate for situations with simple moving shock waves that are dominant in most practical simulations, but may also lead to extremely poor prediction of nonlinear signal speeds for some specific cases, such as bow shocks. As a consequence of the erroneous nonlinear estimates evaluated in Eq. (5), principle assumptions of the underlying HLL-type solver, such as $S_L < S_* < S_R$ are violated by the arithmetic average. Moreover, this fundamental flaw may be hidden by an algorithmic reformulation of the original HLLC Riemann solver, which makes errors due to inaccurate signal speed estimates particularity hard to detect and may lead to unexpected behavior. In contrast to the Einfeldt estimate, both Davis and Toro estimates significantly overestimate signal speeds for strong shocks, which may lead to an increased numerical dissipation. Due to the mentioned facts, we recommend to avoid the arithmetic-average estimate wherever possible, and to apply classical, well-established estimates instead.

CRediT authorship contribution statement

Nico Fleischmann: Conceptualization, Data curation, Investigation, Methodology, Software, Validation, Visualization, Writing - original draft. **Stefan Adami:** Data curation, Project administration, Supervision, Writing - review & editing. **Nikolaus A. Adams:** Funding acquisition, Resources, Supervision, Writing - review & editing.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgements

This project has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (grant agreement No. 667483).

The authors gratefully acknowledge the Gauss Centre for Supercomputing e.V. (www.gauss-centre.eu) for funding this project by providing computing time on the GCS Supercomputer SuperMUC at Leibniz Supercomputing Centre (www.lrz.de).

References

[1] S.K. Godunov, A difference method for numerical calculation of discontinuous solutions of the equations of hydrodynamics, Mat. Sb. 89 (3) (1959) 271–306.
[2] G.-S. Jiang, C.-W. Shu, Efficient implementation of weighted ENO schemes, J. Comput. Phys. 126 (1) (1996) 202–228.
[3] E.F. Toro, Riemann Solvers and Numerical Methods for Fluid Dynamics: A Practical Introduction, Springer Science & Business Media, 2013.
[4] P.L. Roe, Approximate Riemann solvers, parameter vectors, and difference schemes, J. Comput. Phys. 43 (2) (1981) 357–372.
[5] A. Harten, P.D. Lax, B.v. Leer, On upstream differencing and Godunov-type schemes for hyperbolic conservation laws, SIAM Rev. 25 (1) (1983) 35–61.
[6] E.F. Toro, M. Spruce, W. Speares, Restoration of the contact surface in the HLL-Riemann solver, Shock Waves 4 (1) (1994) 25–34.
[7] V. Coralic, T. Colonius, Finite-volume WENO scheme for viscous compressible multicomponent flows, J. Comput. Phys. 274 (2014) 95–121.
[8] M.L. Wong, S.K. Lele, High-order localized dissipation weighted compact nonlinear scheme for shock- and interface-capturing in compressible flows, J. Comput. Phys. 339 (2017) 179–209.
[9] D.P. Garrick, M. Owkes, J.D. Regele, A finite-volume hllc-based scheme for compressible interfacial flows with surface tension, J. Comput. Phys. 339 (2017) 46–67.
[10] N. Fleischmann, S. Adami, N.A. Adams, Numerical symmetry-preserving techniques for low-dissipation shock-capturing schemes, Comput. Fluids 189 (2019) 94–107.
[11] S. Davis, Simplified second-order Godunov-type methods, SIAM J. Sci. Stat. Comput. 9 (3) (1988) 445–473.
[12] B. Einfeldt, On Godunov-type methods for gas dynamics, SIAM J. Numer. Anal. 25 (2) (1988) 294–318.
[13] P. Batten, N. Clarke, C. Lambert, D.M. Causon, On the choice of wavespeeds for the HLLC Riemann solver, SIAM J. Sci. Comput. 18 (6) (1997) 1553–1570.
[14] J.-L. Guermond, B. Popov, Fast estimation from above of the maximum wave speed in the Riemann problem for the Euler equations, J. Comput. Phys. 321 (2016) 908–926.
[15] E. Toro, L. Müller, A. Siviglia, Bounds for wave speeds in the Riemann problem: direct theoretical estimates, Comput. Fluids 209 (2020) 104640.
[16] N. Fleischmann, S. Adami, X.Y. Hu, N.A. Adams, A low dissipation method to cure the grid-aligned shock instability, J. Comput. Phys. 401 (2020) 109004.
[17] S. Gottlieb, C.-W. Shu, E. Tadmor, Strong stability-preserving high-order time discretization methods, SIAM Rev. 43 (1) (2001) 89–112.
[18] E. Johnsen, T. Colonius, Implementation of WENO schemes in compressible multicomponent flow problems, J. Comput. Phys. 219 (2) (2006) 715–732.