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Unresolved Problems by Shock Capturing: Taming the Overheating Problem

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Abstract: The overheating problem, first observed by von Neumann [1] and later studied extensively by Noh [2] using both Eulerian and Lagrangian formulations, remains to be one of the unsolved problems by shock capturing. It is historically well known to occur when a flow is under compression, such as when a shock wave hits and reflects from a wall or when two streams collides with each other. The overheating phenomenon is also found numerically in a smooth flow undergoing rarefaction created by two streams receding from each other. This is in contrary to one's intuition expecting a decrease in internal energy. The excessive amount in the temperature increase does not reduce by refining the mesh size or increasing the order of accuracy. This study finds that the overheating in the receding flow correlates with the entropy generation. By requiring entropy preservation, the overheating is eliminated and the solution is grid convergent. The shock-capturing scheme, as being practiced today, gives rise to the entropy generation, which in turn causes the overheating. This assertion stands up to the convergence test.

Keywords: Numerical Algorithms, Shock Capturing, Exact Contact Discontinuity, Overheating Problem.

1 Introduction

With the enormous advances in numerical algorithms and computer technology, solving a complex three dimensional problems is currently rather common with a desktop computer or local clusters. It is easy to conclude that the basic algorithmic development is no longer necessary, except for the need for physical modeling and mesh generation. On the contrary, this author argues that there are still fundamental problems for which the current *shock capturing approach* have difficulties in providing correct solutions. The objectives of this study are to: (1) revisit some longstanding (open) problems by employing a wide class of modern numerical fluxes, (2) categorize the problems, and (3) to clarify the roots of difficulty and suggest a cure for it.

2 Shock capturing

The shock-capturing method refers to a class of numerical methods that are able to "naturally" yield a shock wave or contact discontinuity as part of a solution, without invoking a special treatment designed to recognize and compute the discontinuities. In contrast, the shock-fitting method explicitly employs in the numerical procedure a mechanism for treating a shock wave by imposing the exact jump; that is, the Rankine-Hugoniot relations. Although at the expense of satisfying the exact jump conditions, the shock-capturing method is by far simpler than its counterpart and has been the basis of nearly all current production codes, whether it be in research or industrial settings. Hence, it is important to sort out what are the long-standing difficulties, determine if they are indeed resolvable within the framework of the shock capturing, and find what correcting formulations should be devised. It must be mentioned that all difficulties to be discussed in this papers have been discretely studied and reported in the past, also listed in the books by LeVeque [3] and Toro [4]. Yet, to the author's knowledge, there is still lacking a dedicated study to compile and sort out the differences of the difficulties. Some of the most known deficiencies derived by the shock-capturing method are the smearing of the discontinuities, especially the moving contact discontinuity, which broadens with time.

The other is the so-called "carbuncle" phenomenon. In this study, we shall employ many popular numerical methods to solve the recognized difficulties, evaluate the performances of these methods, and categorize the difficulties, on the basis of convergence studies so that a difficulty is determined to be a true one, independent of methods, grids, user's own experiences, and parameters. Based on these findings, some clarity about the roots of the difficulties has emerged, suggesting a means for overcoming the problem, but still within the shock capturing framework for its considerable advantages over the shock fitting.

3   Review of past study

In an attempt to have clarity of the causes to the difficulties by the shock-capturing method for the problems mentioned above, an exploratory study was initiated from which some preliminary results and conclusions were presented in [5]. First, it became clear that two different types of difficulties can be delineated, called "fundamental" and "operational." The latter refers to the difficulty that is remediable by changes of operational procedures, such as methods (especially numerical fluxes), time steps, limiters, etc. That is, the correct solution to the problem can be obtained; hence the difficulty is not inherently unresolvable within the shock capturing framework. On the other hand, the fundamental type refers to those still not resolvable under the shock capturing framework. To differentiate whether the problem is fundamental or operation, the convergence test must be upheld for verifying the solution so that a solution is not just a fluke. To this end, numerically stable solutions are ensured in the calculation; thus some numerical fluxes may use a smaller time step than others to stay stable.

Multiple solutions, such as compressive and expansive shocks, are known to exist in nonlinear equations, even though they are numerically stable and grid-converged. The one satisfying physics constraints, in this case the entropy condition, will be expected when judging whether the nature of the problem is fundamental or not, following the mantra, "For a conservative hyperbolic system to converge to a unique weak solution it is necessary that the system is consistent, stable and satisfying entropy condition" [6, 7, 8].

3.1   Carbuncle phenomenon

This is perhaps the most cited shock-capturing difficulty, often illustrated by a supersonic flow over a blunt body or a plane shock wave moving in a constant area channel. It was first reported in the literature by Peery and Imlay [9] and has prompted many studies, fueling many more debates since the appearance of Quirk's study [10]. Some authors even speculate that this phenomenon is physical and incurable [11]. Following the observations in [9, 10], it is understood that the phenomena in question involve an irregular shock profile that deviates from the "expected" known solution by a global length scale, such as the device dimension; see the familiar expose in Fig. 1. Or the solution can go completely wild, leading to a breakdown of the solution, also displayed in Fig. 1 for a plane shock wave moving in a constant-area channel. In either case, it is believed that some sort of instability has initiated and nonlinearity eventually helps limit the growth of the error as in the case shown in Fig. 1. Hence, it is also given a name "shock instability" in [12]. It must be emphasized that no grid convergence can be identified for the carbuncle solution, even if the solution on each grid is stably computed.

Our previous studies [5, 12] have concluded that the carbuncle phenomena problem is an operational one and the observed irregularity is only a numerical artifact produced by some numerical flux methods. This chaotic solution can surface from a normal converged solution after switching to another flux function, see Fig. 2; on the other hand, a normal solution is restored from an ill-behaved solution by switching back to the original flux function, as shown in Fig. 3.

3.2   Overheating problem

The overheating problem was first discussed by von Neumann [1] and later studied extensively by Noh [2] for a shock colliding with and reflecting from a wall. The same phenomenon can be seen also when two opposing streams of fluids collide with each other, creating a contact discontinuity of zero strength if both streams are of equal speed, density and pressure. A common feature in all known shock capturing solutions, central and upwind differencing methods, is an elevated temperature from a correct value, hence termed "overheating." This erroneous temperature appears to be

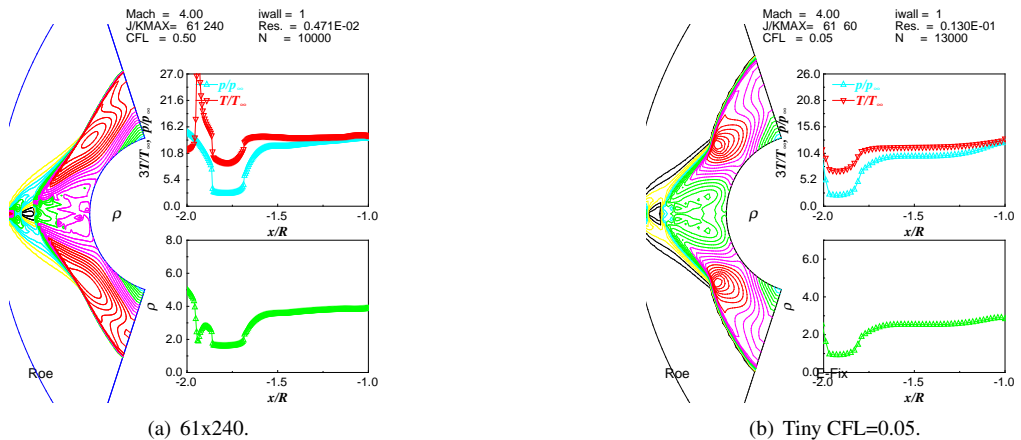(a) 61x240.

(b) Tiny CFL=0.05.

Figure 1: A typical carbuncle solution by the Roe method [13], the solution is not converging by refining the mesh size, extending the outer boundary, or using an extremely small CFL, $M_\infty=4$.
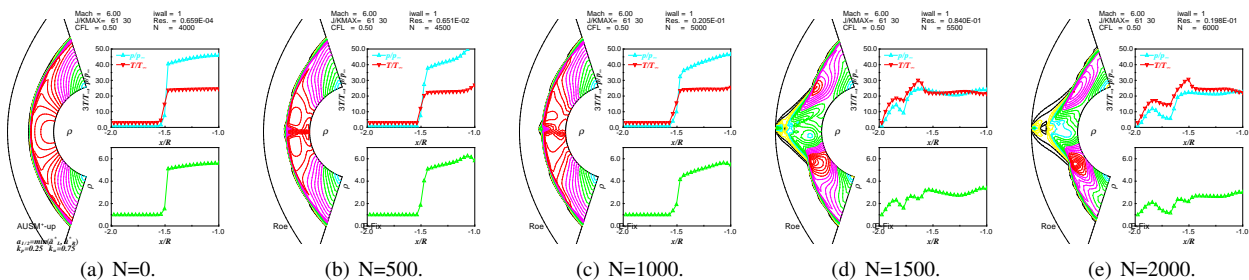

(a) N=0.

(b) N=500.

(c) N=1000.

(d) N=1500.

(e) N=2000.

Figure 2: Evolution of solution by the Roe method, starting from the one converged by AUSM$^+$-up [14], the increment of time steps displayed is 500.

quite stubborn; it was concluded in [5] that no convergence towards the correct value can be established, by refining mesh size, using high order methods, or switching numerical fluxes. Success appears within reach by using a contact-diffusive method, such as the van Leer [15] or HLLE [16] method, which reduces the level of temperature elevation by spreading it over a large area. However, this apparent success causes a significant degradation in the "overheating" phenomenon observed in the rarefying flow, as will be discussed in the next section. An in-depth description about the computed results of the overheating problem associated with the colliding flow can be found in [5].

3.3 Receding flow

The rarefaction created by two receding streams has been used traditionally to test a numerical flux's ability to remain stable when the pressure continues to drop till a vacuum is reached—the so-called positivity preserving property. The Roe scheme [13] is often cited to be lacking this property. For all the flux functions that remain stable, we unexpectedly see a rise in temperature at the center of expansion as depicted in Fig. 4. "Overheating" arises where cooling should happen! As in the case of colliding flows this overheating error is not reduced by refining grid size or increasing order of accuracy. See [5] for a detailed description. Surprisingly, the AUSM$^+$-up method [14] gives a qualitatively correct behavior where the temperature is monotonically decreasing to the lowest value at the center. However, this turns out to be a fluke, because it does not stand up to a convergence test—the center region becomes "overheated" when using a finer grid or second-order accuracy (see Fig. 4(d)). This exercise suggests that a convergence test must be performed whenever possible, especially when a computed solution is in doubt, as in this case and for the carbuncle solution.
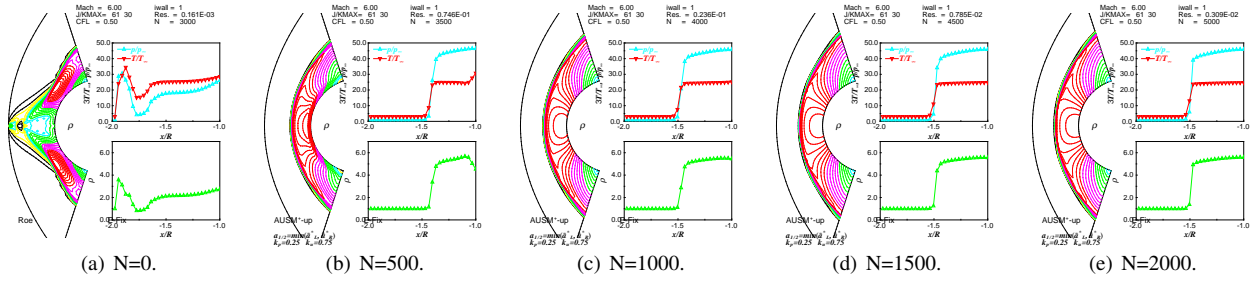
3

(a) N=0. (b) N=500. (c) N=1000. (d) N=1500. (e) N=2000.

Figure 3: Evolution of solution by AUSM$^+$-up, starting from the carbuncular solution by the Roe method, the increment of time steps displayed is 500.

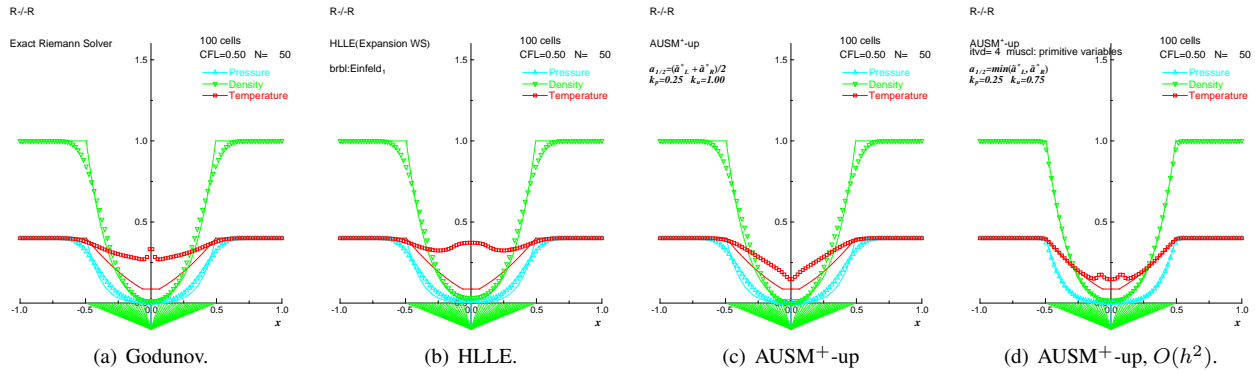(a) Godunov. (b) HLLE. (c) AUSM$^+$-up (d) AUSM$^+$-up, $O(h^2)$.

Figure 4: Receding flows computed on a grid of 100 cells, with the initial condition, $(\rho, p, u)_L = (1.0, 0.4, -2.0)$ and $(\rho, p, u)_R = (1.0, 0.4, 2.0)$,

A case having more features is considered next, with an asymmetric initial condition $(\rho, p, u)_L = (1.0, 2.0, -2.5a_L)$ and $(\rho, p, u)_R = (1.0, 0.5, 2.5a_L)$. This flow is expanding supersonically through a sonic point and contains a contact discontinuity of finite strength. The solutions by the AUSM$^+$-up and HLLE methods with 300 cells are shown in Fig. 5, leading to the following observations: (1) the expansion waves on both fronts are grossly in error, (2) there is a distinctive glitch (here it is different from the entropy jump) at the sonic point, and (3) the region near the contact discontinuity is badly represented, also revealing the "overheating" characteristic. As in the previous case, all methods known to the author lead to a similar behavior, differing only by varying degrees of inaccuracy (see [5]). The diffusive method HLLE gives a larger deviation from the exact solution with a plateau, which is noticeably different from the solutions by the AUSM$^+$-up and Godunov (not included here) methods. Moreover, this plateau persists after employing the MUSCL interpolation with the superbee limiter, even though the solution accuracy in the rest of the domain clearly improves considerably, see Fig. 5. However, the "overheating" remains as formidable to defeat as in the previous receding flow problem, perhaps even more so now because the need for capturing the nondiminishing contact discontinuity must also be met.

The overheating is clearly the creation of a numerical method. This difficulty is encountered by every upwind method that the author has tested [5], and moreover, the problem persists irrespective of using many possible operational variations, such as grid size, time step, high-order interpolation and limiters, time-stepping procedures, etc. Hence, the overheating problem in both colliding and receding flows is classified as an open problem; the problem from receding flow may have an entirely different root cause than the one from colliding flow.
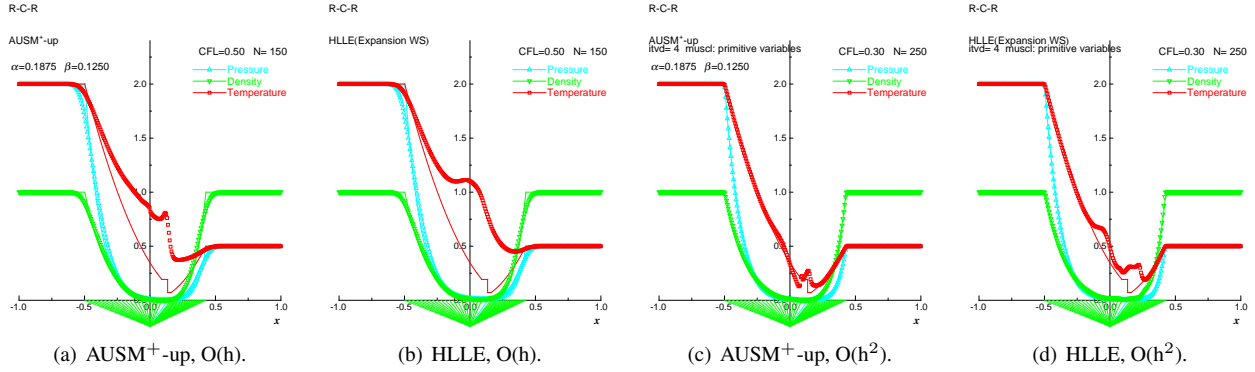
4

(a) AUSM$^+$-up, O(h). (b) HLLE, O(h). (c) AUSM$^+$-up, O(h^2). (d) HLLE, O(h^2).

Figure 5: Comparison of AUSM$^+$-up and HLLE solutions for the receding flow on a grid of 300 cells. $(\rho, p, u)_L = (1.0, 2.0, -2.5a_L)$ and $(\rho, p, u)_R = (1.0, 0.5, 2.5a_L)$.

4 Cause of overheating: entropy generation

The overheating problem occurring in the receding flow is more problematic in the sense that the temperature field is clearly incorrect, albeit the pressure and density distributions at least appear to behave correctly. The key implication is the rate of change in the internal energy as is calculated from the energy equation is inconsistent with physics. Figure 6 provides details of the changes in the internal energy profiles at various time steps N, revealing three distinct events: (1) overheating establishes immediately after the flow begins, (2) a brief period during which the centered region becomes "overcooled" (N=20), and finally (3) stable overheating that remains. Examination of the entropy evolution, shown in Fig. 7, astonishingly reveals an unphysical behavior that by and large corresponds to that of the internal energy.[1] We see that (1) the entropy is increased, even in this smooth flow in the first moment at the center, which clearly violates the second law of thermodynamics, and (2) this entropy violation continues to spread spatially. Furthermore, Fig. 8 shows that the entropy peak at the center reaches a maximum value and then it quickly relaxes to a saturated value. Also in the same figure, this saturated value is found to be rather insensitive to the number of mesh points used. This explains why the overheating is not shrunk by changing the order of accuracy or mesh size. It strongly suggests that in order to resolve this unphysical overheating problem in the receding flow, preservation of the entropy is the key.
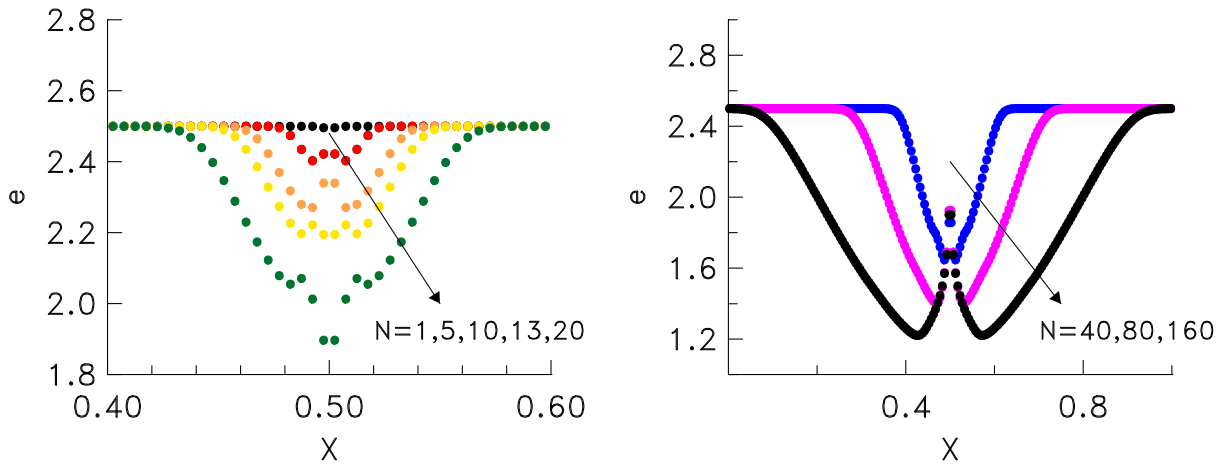

Figure 6: Evolution of internal energy, plotted at various time slices.

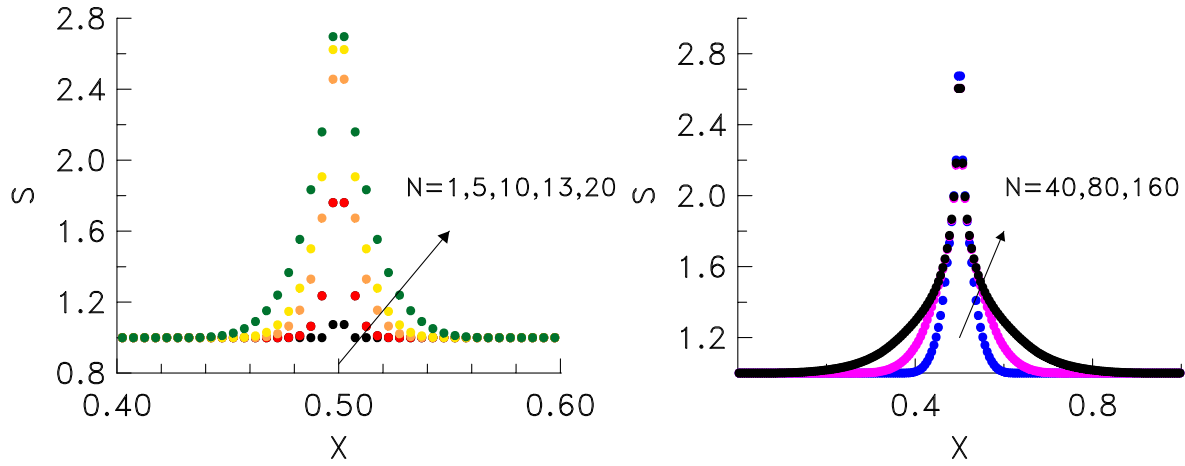[1]Here, the nondimensional entropy function S is defined as $S = \ln(p/\rho^\gamma)$.

Figure 7: Evolution of entropy at various time slices.
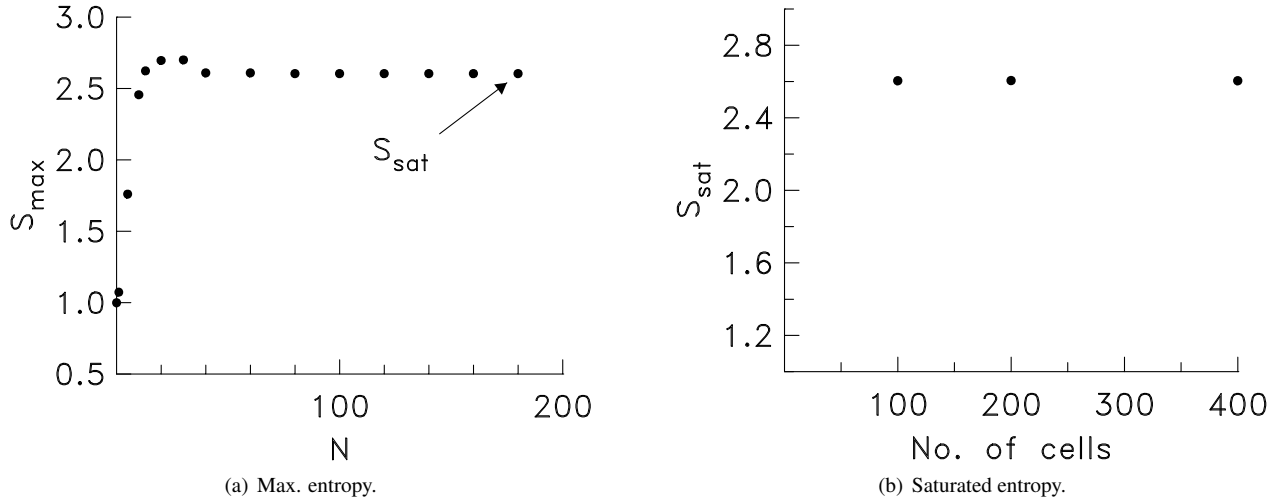

(a) Max. entropy.

(b) Saturated entropy.

Figure 8: (a) Evolution of maximum entropy on the grid of 200 cells and (b) Saturated entropy on different grids.

As the entropy must remain constant for this adiabatic receding flow where no shocks exist, one can justify to solve this problem using the isentropic condition in lieu of the energy equation. The results are given in Fig. 9. They clearly confirm the above conjecture that the violation of entropy condition is the root of the overheating in the receding flow and that the inability of the shock-capturing schemes, as being practiced today, is the cause of this entropy violation. This assertion is further validated by the convergence test.

5   Concluding Remarks and Future Work

Interest in studying outstanding unresolved problems computed within the shock-capturing framework is continued in this paper. To help sort out the level of difficulties encountered, they are categorized into two: (1) operational and (2) fundamental difficulties. The well-known example of the carbuncle problem belongs to the first group because the chaotic behavior can be eradicated by changing operational procedures, such as grid size, time step, high-order interpolation and limiters, time-stepping procedures, etc. The vindication of this classification must be confirmed against the convergence test so that a conclusion is not merely based on a singular solution. The convergence test is strongly advocated as an ultimate and necessary criterion to resolve disagreements in findings and conclusions.
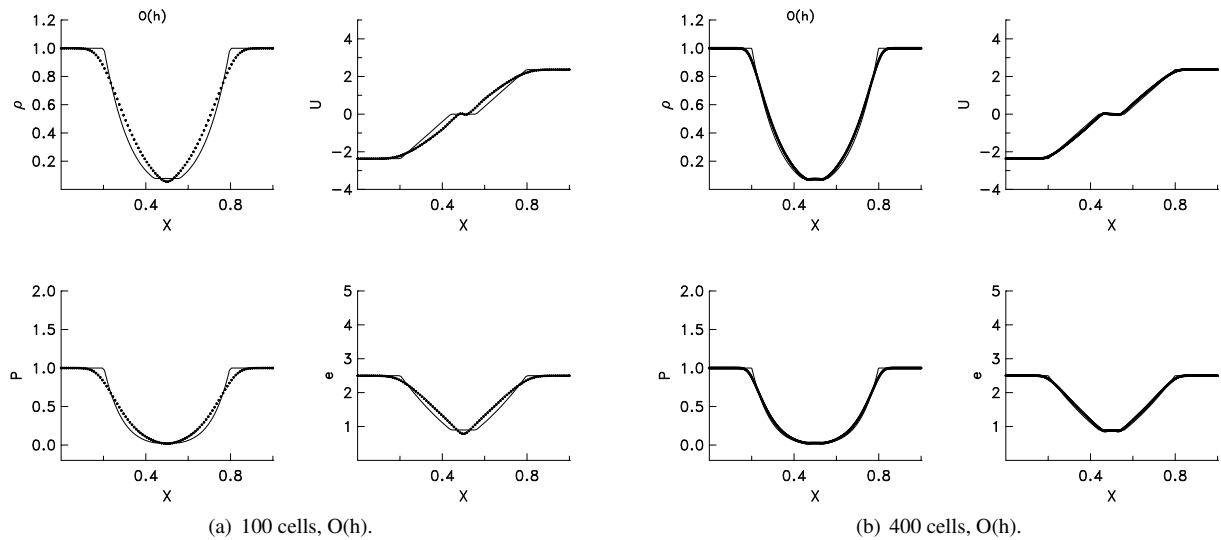
(a) 100 cells, O(h).   (b) 400 cells, O(h).

Figure 9: Solution of the receding flow after satisfying the constant entropy-preservation condition on 100-cell and 400-cell grids, showing grid convergence.

The fundamental difficulty is classified as an open problem. In this study, we conclude that the overheating problem, whether resulting from two colliding or receding streams, is the open problem still unresolved by the current shock-capturing methods. In particular, the overheating in the receding flow problem is not just an unpleasant glitch, but it is also unphysicalheating in rarefying condition! Through a systematic investigation of the internal energy evolution, we discovered that the overheating strongly correlates with the generation of entropy. We conclude that the cause of the overheating is a numerical one, rooted in the inaccuracy introduced in solving the energy equation. The overheating disappears if the entropy-preserving condition is enforced, in lieu of solving the energy equation. Moreover, the assertion of the connection of the entropy violation and the overheating stands up to the convergence test.

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