Computational Accuracy and Mesh Reynolds Number

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The steady-state Burgers' equation $uu_x = (1/\text{Re}) u_{xx}$ ($0 \le x \le 1$) with boundary values u(0) = 0 and u(1) = -1 is employed as a model equation for fluid dynamics. It is shown how different conservative discretizations of the nonlinear term uu_x govern the discretization error in computational results, especially when the mesh Reynolds number Re Δx is not small. For a particular choice of the nonlinear discretization, the maximum error in the computed result can attain a value at some fairly large Re Δx comparable to that expected at a much smaller Re Δx . The formal order of accuracy of an algorithm, in terms of either Δx or Re Δx , does not reflect the accuracy of computational results, especially when the mesh is coarse.

1. INTRODUCTION

This paper employs the nonlinear, steady-state Burgers' differential equation $uu_x = (1/\text{Re}) u_{xx}$ as a model for viscous fluid flow, and investigates solutions of the corresponding nonlinear finite difference equations. The term u_{xx} is represented by the standard centered difference $(U_{j+1} - 2U_j + U_{j-1})/\Delta x^2$, and the nonlinear term is replaced by the second order accurate approximation

$$\left(rac{\gamma}{2+\gamma}
ight)rac{U_{j}(U_{j+1}-U_{j-1})}{2\Delta x}+\left(rac{2}{2+\gamma}
ight)rac{U_{j+1}^{2}-U_{j-1}^{2}}{4\Delta x}\,.$$

Additionally, in Section 5 a first order accurate approximation of uu_x is used for comparison.

By comparing the discrete solutions of the nonlinear difference equations with an exact differential solution, errors are evaluated as functions of the various parameters of the problem. These parameters include both those introduced by the process of discretization, such as the mesh size, and those presented by the physical problem itself, such as the Reynolds number. We obtain analytic (as opposed to computational) results for this simple nonlinear model problem which give functional relationships between the properties of the difference solution and the problem parameters. A forthcoming extension of this analysis will present similar results for more complicated gasdynamic model systems.

This study concentrates on errors due to discretization alone. Boundary errors are avoided by exactly specifying boundary values. We study only difference formulations generated by a class of conservative difference algorithms, so that there is no accumulation of local discretization error in the interior of any combination of computational cells. This allows the extension of the Stokes theorem to secure physical conservation relations over arbitrary volumes in the difference formulation. This analog of the Stokes theorem is crucial in our analytic treatment of the nonlinear difference solutions. These difference solutions differ from the differential solution only because of the (nonaccumulated) error of discretization.

This error of discretization is often identified as the "local truncation error" with some "formal order of accuracy" based on the truncated residue in the Taylor series approximation of the difference equations. Such terms can only be meaningful when computing with a sufficiently small mesh size. Otherwise, difference quotients may fail to reasonably approximate derivatives, and the Taylor expansions involved in the formal definitions of accuracy become meaningless. This is especially true for oscillatory difference solutions of complicated problems when we are forced to use a rather coarse mesh under the storage capacity and speed limitations of currently available computing machines. We show that the formal order of accuracy of a difference scheme does not reflect the magnitude of discretization error for such problems, and we identify those parameters which do reflect this error.

In the following, we give exact solutions of the nonlinear difference system for certain special values of the Reynolds number. Otherwise, we construct approximate solutions of the difference system by retaining the nonlinearity where crucial. Such approximate analytic solutions are found to agree well with those obtained by direct digital computation. The crucial influence of the mesh Reynolds number Re Δx on the accuracy of the computation, based on a given algorithm, can then be analytically established. We identify the outstanding advantage of a conservative difference formulation in providing an optimal Re Δx of fair size for minimizing the maximum error E_{∞} . The sensitive dependence of E_{∞} on slight variations in the difference algorithm, particularly the method of differencing nonlinear terms, is demonstrated We hope that constructive suggestions from the present results will be helpful for computational solutions of the nonlinear partial differential equations of fluid mechanics.

2. NONLINEAR MODEL PROBLEM

A. Differential Model

The partial differential equation

$$w_t + (w - c) w_z = \nu w_{zz} \tag{1a}$$

reduces in the steady-state $(t \rightarrow \infty, \partial/\partial t \rightarrow 0)$ to

$$(w-c)w_z = vw_{zz}, \qquad (1b)$$



FIG. 1. Model problem in physical space.

which has the exact solution

$$w(z) = c - \frac{\alpha \, \Delta w}{2} \tanh\left(\frac{\alpha \, \Delta w}{4\nu} \cdot z\right), \tag{1c}$$

where w(z = 0) = c, $w(z = \pm L) = c \mp \Delta w/2$, $w(z = \pm \infty) = c \mp \alpha \Delta w/2$ and α satisfies $\alpha \tanh(\alpha \Delta w L/4\nu) = 1$. Here Δw , c, and ν (a kinematic viscosity) are given constants. We interpret (1c) as defining a symmetric transition region of length 2L, centered about w = c, representing a jump in the value of w by the amount Δw under the effective pressure gradient $-cw_z$ (Fig. 1). The transformation

$$u = \frac{w-c}{(\Delta w/2)}, \qquad x = z/L, \qquad \tau = \frac{(\Delta w/2)}{L}t$$
 (2)

reduces Eq. (1a) for w to the time-dependent Burgers equation

$$u_{\tau} + uu_{x} = \frac{1}{\operatorname{Re}_{L}} u_{xx} \,. \tag{3a}$$

Here $\operatorname{Re}_L = (\Delta w/2)L/\nu$ is a Reynolds number based upon a characteristic velocity $\Delta w/2$ equal to half of the jump magnitude Δw , and a characteristic length L equal to half of the computational field size 2L over which the velocity jump is accomplished.

In the steady-state, Burgers' Eq. (3a) reduces to

$$uu_x = \frac{1}{\operatorname{Re}_L} u_{xx}, \qquad (3b)$$

which has the exact solution

$$u(x) = -\alpha \tanh\left(\frac{\alpha \operatorname{Re}_{L}}{2} \cdot x\right)$$
(3c)

satisfying the boundary conditions

$$u(x=0) = 0,$$
 (3d)

$$u(x=1) = -1.$$
 (3e)

Equation (3b), together with boundary conditions (3d), (3e), constitutes our differential model describing the jump condition. We have taken advantage of the symmetry of the differential solution (3c) to consider only "half" of the transition profile, $-1 \le u \le 0$ (Fig. 2A).

The existence of this steady-state solution (3c) indicates the presence of an unchanging wave front propagating with the average velocity c in the physical space z. The origin of the transformed coordinate x propagates with the wave.



FIG. 2. Typical difference solutions (with method of approximate difference solution schematically indicated). (A) Smooth (Re $\Delta x \leq 1$). (B) Oscillatory ($1 \leq \text{Re } \Delta x < \text{Re}^* \Delta x$). (C) "Exact" (Re $\Delta x = \text{Re}^* \Delta x$). (D) Oscillatory (Re $\Delta x > \text{Re}^* \Delta x$).

B. Difference Model

To obtain the difference equation, the x-coordinate is discretized as $x = j \Delta x$ (j = 0, 1, 2, ..., J) so that $J \Delta x = 1$, and the mesh function is taken as $U_j = U(j \Delta x)$. The terms of Eq. (3b) are discretized with formal second order accuracy as

$$u_{xx} = \frac{U_{j+1} - 2U_j + U_{j-1}}{\Delta x^2},$$

$$uu_x = \left(\frac{u^2}{2}\right)_x = \left(\frac{\gamma}{2+\gamma}\right) \frac{U_j(U_{j+1} - U_{j-1})}{2\Delta x} + \left(\frac{2}{2+\gamma}\right) \frac{(U_{j+1}^2 - U_{j-1}^2)}{4\Delta x},$$
(4)

where the latter difference quotient (with γ replacing *a* introduced in [1]) represents a weighted average of centered difference approximations of the convective form uu_x and the differentially equivalent divergence form $(u^2/2)_x$. Thus the difference equation system representing (3b) is

$$U_{j+1}^{2} + \gamma U_{j}(U_{j+1} - U_{j-1}) - U_{j-1}^{2}$$

= $\frac{2(2 + \gamma)}{\text{Re }\Delta x} [U_{j+1} - 2U_{j} + U_{j-1}], \quad j = 1, 2, ..., J - 1,$ (5a)

and the boundary conditions representing (3d), (3e) are

$$U_0 = 0 \quad \text{and} \quad U_J = -1. \tag{5b}$$

It can be seen from (5a) that difference solutions, like differential solutions, are always symmetric about U = 0. By considering only half of the profile in our model we have, however, tacitly assumed that the whole profile is computed with an odd number of mesh points. Only in this case is there in fact a mesh point exactly at the symmetry point of the whole profile.

C. Comments on the Models

The effects of discretizing the differential problem are reflected by the mesh size Δx and the number of mesh points J + 1, where $J \Delta x = 1$. The parameter Re $\Delta x =$ $(\Delta w/2)L\Delta x/\nu = (\Delta w/2)\Delta z/\nu$ is termed the "mesh Reynolds number." This important parameter [1-3] reflects the physical characteristics of the flow $(\Delta w/2, \nu)$, the computational field size (L), and the discretization effect of the mesh size $\Delta x = 1/J$. Re Δx . and not Δx alone, stands as a parameter in the difference equations and measures the fineness of the computational mesh relative to the steepness of the gradient one wishes to compute. If, for example, the fluid Reynolds number Re_L in model (3c) is doubled (say by halving ν), the maximum gradient $|U_x(x=0)| \sim \text{Re}_1/2$ is doubled. Should Δx remain unchanged, there will be roughly half as many mesh points in the narrower transition region near x = 0. In order to maintain the same resolution, it is necessary to halve Δx , whereby the original value of Re Δx is restored. Thus Re Δx is the appropriate parameter reflecting computational resolution. A small value of Re Δx means a fine mesh, while a large value indicates a coarse mesh. Attempts to improve computational accuracy through mesh refinement (i.e., decreasing Δx for a fixed Re₁) will be interpreted through this parameter Re Δx . It is emphasized that Re Δx as defined here is based on the characteristic velocity jump $(\Delta w/2)$ of the model transition region, and not (as often misconstrued) on the upstream reference velocity or local instantaneous convective velocity.

The particular form of nonlinear differencing (4) was specifically constructed to yield a conservative difference system, so that the finite difference analog of Stokes' theorem may be applied [4]. This property is crucial to our analysis in Section 4. The parameter γ introduced in (4) is an arbitrary discretization parameter. For any choice of γ , algorithm (4) is conservative and formally second order accurate. Different

choices of γ result only in different Taylor series residues, all of which are formally of order $(\Delta x)^3$ or higher. Such difference algorithms which differ formally only in higher order terms are shown to lead to quite different solutions when the limit $\Delta x \to 0$ is *not* taken.

The difference equations system (5a) will also result if algorithm (4) is employed to discretize Eq. (1b) and transformation (2) is then applied. Thus the difference solution of (5a), (5b) truly solves the symmetric half of the transition profile of our model flow problem depicted in Fig. 1.

For given values of Re Δx and γ , the system of coupled nonlinear algebraic equations (5a), (5b) has a large number of solutions, more than one of which may be realvalued. At finite Re Δx , the various solutions may differ considerably, even if they all converge to the same limit as Re $\Delta x \rightarrow 0$. The central question is whether any or all of such difference solutions constitute "good" approximations to the differential solution when Re $\Delta x \geq O(1)$. Since computations at Re $\Delta x \geq O(1)$ do often provide "decent" approximations except in small regions where computational oscillations may be excessive, the present study focuses on those solutions of (5a), (5b) which are "decent," "well-behaved" solutions in the above sense, and on the effects of the representative computational parameters Re Δx and γ upon the errors in such computed solutions at Re $\Delta x \geq O(1)$.

3. EXACT NONLINEAR DIFFERENCE SOLUTION

We now describe a family of solutions of the nonlinear difference system, Eqs. (5a), (5b), for the special mesh Reynolds numbers

Re
$$\Delta x = \operatorname{Re}^* \Delta x = \frac{2(2+\gamma)}{(1+\gamma)}$$
. (6a)

At this value Re* Δx , the solution of system (5a) subject to boundary values (5b), i.e., $U_0 = 0$ and $U_J = -1$, is given as

$$U_0 = 0,$$

 $U_j = -1, \quad j = 1, 2, ..., J.$
(6b)

These solutions, depicted in Fig. 2C, exhibit no oscillation and are good approximations (especially at large Re Δx) to the differential solution (3c).

These solutions are remarkable in that they render an abrupt transition (within 1-2 mesh spacings) without inducing oscillations into the computed flow field away from the transition region. They are highly desirable *if the detailed structure within such transition regions is not of particular concern*, as for shock waves in an inviscid field. Indeed, when the shock thickness is less than the computational mesh size Δx , this abrupt transition is the best one could hope for.

It is noteworthy that the exact solution (6b) of the difference system occurs at different values of Re Δx for different choices of γ in differencing the nonlinear term. Thus with $\gamma = 0$ and $\gamma = \infty$ we have Re* $\Delta x = 4$ and Re* $\Delta x = 2$ respectively, and we obtain Re* $\Delta x \to \infty$ as $\gamma \to -1$. From the point of view of constructing difference algorithm (4), there is no obvious reason to prefer any particular choice of γ . However, if Re Δx is known a priori, the choice $\gamma = \gamma^* = (\text{Re } \Delta x - 4)/(2 - \text{Re } \Delta x)$ is "optimal" in the sense of yielding a nonoscillatory difference solution even if Re Δx is fairly large.

4. Approximate Solution of Nonlinear Difference Equations

This section outlines a method for constructing coarse mesh solutions of difference system (5a), (5b) for arbitrary combinations of the parameters γ , Re Δx , and J (especially for fairly large Re Δx and J). Linearized perturbation approaches for solving a nonlinear difference system, such as the methods of Strang [5] and Cheng [1], require expansions in terms of a small parameter. These methods are therefore not useful in the present endeavor.

The crucial step in the present analysis is to sum both sides of (5a) from j = 1 to j = J - 1, and rearrange to get

$$U_{0}^{2} + U_{1}^{2} + \gamma U_{0}U_{1} - \frac{2(2+\gamma)}{\text{Re }\Delta x}(U_{1} - U_{0})$$

= $U_{J-1}^{2} + U_{J}^{2} + \gamma U_{J-1}U_{J} - \frac{2(2+\gamma)}{\text{Re }\Delta x}(U_{J} - U_{J-1}).$ (7)

This summation is conveniently carried out since the difference algorithm generating (5a) is strictly conservative, and thus flux terms at interior cell boundaries cancel identically. The summation process is analogous to the application of Stokes' theorem to the differential problem. By employing boundary conditions (5b) and defining $\epsilon = U_J - U_{J-1}$, Eq. (7) can be solved for U_1 to give

$$U_1 = \left(\frac{2+\gamma}{\operatorname{Re}\,\Delta x}\right) - (2+\gamma)^{1/2} \left[1 + \frac{2+\gamma}{(\operatorname{Re}\,\Delta x)^2} + \epsilon \left(1 - \frac{2}{\operatorname{Re}\,\Delta x}\right) + \frac{\epsilon^2}{2+\gamma}\right]^{1/2}.$$
(8)

Here, as in the following, the appropriate sign is chosen in the quadratic formula to obtain the difference solution which can possibly serve as a reasonable approximation to (3c).

For given values of Re Δx and γ , U_1 is determined by (8) if ϵ is known. Now $|\epsilon|$ can be made as small as desired by taking J sufficiently large. This can be justified by a conceptually simple but algebraically complicated method of regions which retains the crucial nonlinearity only near x = 0 where the gradient of the genuine solution is large. This method is outlined schematically in Fig. 2; the details are given

in [7]. An outstanding result of this analysis is that $|\epsilon|$ is very small for $J \gtrsim 10$ or 20 when Re Δx assumes values common in practice (O(10)). Thus when the flow feature in a practical computation is resolved by 10 to 20 or more mesh points, we may for all practical purposes take $\epsilon = 0$. The error in the results of computation with a given algorithm of discretization (given γ) will then be essentially a function of Re Δx only.

Specifically, taking $\epsilon = 0$ in (8) gives

$$U_{1} = \left(\frac{2+\gamma}{\text{Re }\Delta x}\right) - (2+\gamma)^{1/2} \left[1 + \frac{2+\gamma}{(\text{Re }\Delta x)^{2}}\right]^{1/2}.$$
 (9)

The value of U_2 can now be readily found from the nonlinear difference equation (5a) at j = 1 (with the boundary condition $U_0 = 0$) by solving

$$U_{2}^{2} + \left[\gamma U_{1} - \frac{2(2+\gamma)}{\text{Re }\Delta x}\right] U_{2} + \frac{4(2+\gamma)}{\text{Re }\Delta x} U_{1} = 0.$$
(10)

If desired, values of U at successive mesh points can also be determined. As may be expected (and is verified by test computations), the maximum error occurs at either j = 1 or j = 2 in the region of maximum gradient. Thus knowledge of U_1 and U_2 is sufficient to compute the error in the maximum norm. Defining the pointwise errors as

$$e_j = |u(j\Delta x) - U_j|, \quad j = 1, 2$$
 (11)

the maximum error is then

$$E_{\infty}(\gamma, \operatorname{Re} \Delta x) = \max(e_1, e_2). \tag{12}$$

Here u is the differential solution (3c) and U is given analytically by Eqs. (9) and (10).

At large but finite Re Δx , the errors defined in (12) can be easily computed for any fixed γ ; the results of such computation are displayed in Fig. (3). These results have been confirmed by direct digital computation with various time-dependent algorithms (summarized in [6]) which reduce to (5a), (5b) in the steady-state. The maximum discretization error E_{∞} committed by the difference solution is given as a function of Re Δx , where each curve is labeled with a value of the discretization parameter γ and the corresponding value of Re^{*} Δx given by (6a). For a given γ , the error curve shows a conspicuous minimum at a value of Re Δx slightly less than Re^{*} $\Delta x = 2(2 + \gamma)/(1 + \gamma)$. This is expected since at large Re Δx , the differential solution (3c) is essentially $u(j \Delta x) = -1$ for $j \ge 1$; thus the exact difference solution, the choice of $\gamma = \gamma^* = (\text{Re } \Delta x - 4)/(2 - \text{Re } \Delta x)$ is very nearly optimal. We reiterate that this type of difference solution does not resolve the detailed structure of the transition region, but is instead an abrupt jump solution with the desirable feature of generating no computational oscillations away from the transition region.

The mesh Reynolds number Re Δx is a composite parameter which depends on the linear dimension L of the computational field, on the mesh size $\Delta x = 1/J$, and on the characteristic velocity jump being computed. Computation at a given Re Δx can be achieved with different combinations of the field size L and the number of mesh points J + 1. The presumed convergence of the computation at sufficiently small Δx or Re Δx naturally suggests that repeated computations at successively refined meshes will improve computational accuracy. Such mesh refinements can be accomplished by increasing J (decreasing Δx) until the computer limitations of storage, speed, and cost are encountered, and then by reducing the computational field size L. However, a practical lower limit on Re Δx will be reached due to the increasing difficulty in specifying boundary conditions as the boundaries of the field of computation come closer to the flow feature of interest. Thus, the Re Δx of practical computations will generally be appreciably larger than unity. Even without boundary errors, Fig. 3 shows that when $\operatorname{Re} \Delta x \leq \operatorname{Re}^* \Delta x$, it is quite possible to decrease $\operatorname{Re} \Delta x$ (by decreasing Δx and/or L) and obtain a worse solution. (This does not occur if Re $\Delta x \leq 2$ where the error bound $|E_{\infty}| \leq 0.03$ (Re Δx)² given in [1] is very good, but such values can hardly be reached in practical computation.) Thus for the coarse mesh computations, it is highly desirable to have some idea of Re* Δx in order to identify an optimal solution during the process of mesh refinement.



FIG. 3. Error committed by nonlinear difference solution for various γ , J large.

5. FIRST ORDER SCHEMES

The results in Fig. 3 show clearly that for coarse meshes, the error does not vary as $(\text{Re } \Delta x)^2$ as suggested by the formal second order accuracy of the difference algorithms. To further illustrate this failure of the formal order of accuracy to predict the magnitude of computational errors, we briefly investigate the effect of discretizing the term uu_x with formal first (rather than second) order accuracy. Consideration

is restricted to the following two cases, both in divergence form $(u^2/2)_x$, namely,

forward (down gradient) differencing
$$\left(\frac{u^2}{2}\right)_x \sim \frac{1}{2} \cdot \frac{U_{j+1}^2 - U_j^2}{\Delta x}$$
, (13a)

backward (up gradient) differencing
$$\left(\frac{u^2}{2}\right)_x \sim \frac{1}{2} \cdot \frac{U_j^2 - U_{j-1}^2}{\Delta x}$$
. (13b)

All first order schemes for discretizing the convective term uu_x , such as $U_j(U_{j+1} - U_j)/\Delta x$, result in nonconservative difference systems and thus prevent the convenient summation of the difference system which is crucial to our analysis. The nonlinear difference systems resulting from employing (13a) or (13b) in model equation (3b) are respectively

$$U_{j+1}^{2} - U_{j}^{2} = \frac{2}{\operatorname{Re} \Delta x} \left(U_{j+1} - 2U_{j} + U_{j-1} \right)$$
(14a)

and

$$U_{j}^{2} - U_{j-1}^{2} = \frac{2}{\operatorname{Re} \Delta x} (U_{j+1} - 2U_{j} + U_{j-1}).$$
(14b)

Equations (14a) and (14b) hold for j = 1, 2, ..., J - 1, and are subject to boundary conditions (5b). Before presenting the results, we wish to emphasize that systems (14a) and (14b) are not invariant with respect to a reversal of the positive x- and U-directions, so that these results are not applicable for a computation of the "whole" profile shown in Fig. 1.

The exact nonlinear difference solution (6b) exists for the difference systems (14a) and (14b) when Re* $\Delta x = \infty$ and Re* $\Delta x = 2$, respectively. Proceeding as in Section 4 by summing (14a) and (14b) from j = 1 to j = J - 1, invoking the boundary conditions $U_0 = 0$ and $U_J = -1$, taking $\epsilon = 0$ (i.e., $U_J = U_{J-1}$), and solving for U_1 gives respectively

$$U_1 = \frac{1}{\operatorname{Re} \Delta x} - \left(1 + \frac{1}{(\operatorname{Re} \Delta x)^2}\right)^{1/2}$$
(15a)

and

$$U_1 = -\operatorname{Re} \Delta x/2. \tag{15b}$$

The errors, defined in (12) and computed from (15a) and (15b) (the maximum error always occurs at j = 1), are displayed in Fig. 4. The error curve for forward differencing was verified by actual computation with the Cheng-Allen scheme; for backward differencing, computation was unstable at large Re Δx (as expected from (15b)).

The following features are apparent:

(i) The behavior of the forward difference solution is similar to that of the formally second order difference solution with $\gamma = -1$. Indeed, Eq. (15a) is identical with (8) when $\gamma = -1$ and $\epsilon = 0$. Thus for J large ($|\epsilon|$ small), the behavior of the

first order scheme (13a) is substantially the same as that of the second order scheme with $\gamma = -1$.

(ii) Difference solutions with small error can be obtained at large Re Δx if differencing is always performed in the "correct" direction. We note that this direction is not always "upwind," since the "upwind" direction can be reversed by the addition of the mean velocity c. The correct direction should be "down the magnitude of the gradient," which is often not known a priori.



FIG. 4. Error committed by first order difference solutions.

6. CONCLUSIONS

The present analytic study of the solutions of the system of nonlinear difference equations describing the transition from one uniform flow velocity to another yields the following results that may be useful for guiding the computational solution of related practical problems:

(i) With a group of formally second order accurate, strictly conservative difference algorithms, it is possible to obtain computational solutions with an error (based on the maximum norm) $E_{\infty} \leq 10\%$ at fairly large mesh Reynolds numbers (Re $\Delta x \geq 10$) by choosing the discretization parameter γ in the range $-1 \leq \gamma \leq 0$. If we compute at Re $\Delta x = 2(2 + \gamma)/(1 + \gamma)$, E_{∞} may be less than 1%, comparable with error values normally expected for computations at much smaller Re $\Delta x \leq 1$.

(ii) The errors in computational results with formally second order accurate algorithms and coarse meshes vary widely, and do not increase as Δx^2 or $(\text{Re }\Delta x)^2$. Furthermore, the first order accurate algorithm (13a) can provide essentially the same solution as does the second order algorithm with $\gamma = -1$; such results can be either better or worse than those afforded by other formally second order schemes. Thus the formal order of accuracy of a difference algorithm may not reflect the magnitude of computational errors. The accuracy of computed results is a complicated function of the parameters Re Δx and γ and of the conservative property of the difference algorithm. Mesh refinement at large Re Δx need not lead to a more accurate solution.

(iii) Similar results for more general gasdynamic models will be reported separately.

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