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Technical Notes

Effect of Shock-Capturing Errors on Turbulence Statistics

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Nomenclature

C	=	method-dependent constant
h, h_i	=	grid spacing
k_i, k	=	wave-number vector and magnitude
k_0	=	wave number of peak energy
R_{ij}	=	Reynolds stress tensor, $\widetilde{u_i'' u_j''}$
r	=	shock compression ratio, ρ_d/ρ_u
S	=	mean compression rate in rapid distortion theory
u_i	=	velocity
γ	=	gas constant (taken as 1.4)
δ	=	numerical shock thickness
δ_{ij}	=	Kronecker delta
ϵ_{ij}	=	error in postshock R_{ij}
κ	=	normalized wave number, k/k_0
ν	=	kinematic viscosity
ρ	=	density
τ	=	normalized time, $St/\ell_n(r)$
$\tilde{}$	=	Favre average
$\hat{}$	=	Fourier component

Subscripts

u, d	=	upstream or downstream of shock
1, 2, i, j	=	tensor indices

Introduction

THE presence of shock waves is an important feature of high-speed fluid flows. At realistic Mach and Reynolds numbers, the shock thickness is vanishingly small; therefore, the only realistic computational approach is to either treat the shock as an interface (shock fitting) or to use numerics that smear the shock over a few grid points while predicting the correct shock jumps (shock capturing). There are many shock-capturing numerical methods in the literature, but (as is well known) they must necessarily be first-order accurate in the L_1 norm when applied to a shock. This is easily understood by the facts that 1) the shock will occupy a constant number of grid points regardless of the grid spacing, and 2) there will always be a pointwise error proportional to the shock jump due to the smearing. However, it is not clear that this definition of the error is the most relevant in practice. Common turbulence statistics (e.g., Reynolds stresses or vorticity variances) are insensitive to phase information; therefore, the convergence of turbulence statistics is not necessarily a first-order process.

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The present work is focused on direct numerical simulation (DNS) or large eddy simulation (LES) of shock/turbulence interactions. One key feature of such interactions is the amplification of Reynolds stresses and vorticity. There are several potential sources of error away from the shock, including insufficient grid resolution or excessive numerical dissipation; both of these are well documented in the literature (cf., Lee et al [1] for a comparison of shock-capturing versus shock-resolving calculations and Larsson and Lele [2] for a general error discussion). An additional source of error is the numerical damping at the shock, where there must necessarily be significant numerical viscosity. This error affects both DNS and LES, and it has not (to the author's knowledge) been analyzed in the literature.

The objective of this Note is to analyze the error at the shock and develop an approximate relationship between the shock-normal grid spacing, the numerical method, and the error in the postshock turbulence statistics. A key consideration has been to strike a balance between analytical simplicity and application relevance. At the outset, the error estimate is required to be valid for broadband three-dimensional (3-D) turbulence to ensure relevance to applied LES and DNS. To simplify the analysis, only isotropic upstream turbulence and normal shock waves are considered here. These are obvious limitations, but the general conclusions should be applicable to anisotropic turbulence and/or oblique shocks as well. In addition, rapid distortion theory (RDT) is used to approximate the turbulence modification due to the shock, despite its well-known shortcomings in describing shock/turbulence interactions.

Subscripts 1, 2, i, and j denote tensor indices, while subscripts u and d denote whether a point is upstream or downstream of the shock. For example, $k_{1,u}$ is the streamwise (shock normal) wave number upstream of the shock, whereas $u_{2,d}$ is the transverse velocity downstream of the shock.

Error Model

Shock-capturing schemes work by adding numerical diffusion that smears the shock over a few grid points, thereby allowing it to be captured by the numerical method. A simple balance of convective and viscous terms (in the Navier–Stokes equations) in a frame where the shock is stationary yields $\rho u_1 \Delta u_1/h \sim \rho\nu\Delta u_1/h^2$, where Δu_1 is the jump in velocity at the shock. This gives $\nu \sim u_1 h$, which shows that shock capturing must necessarily introduce dissipation that depends linearly on the grid spacing (i.e., first-order accurate).

In the present Note, the modification to an incoming signal u is idealized in two steps: 1) the exact modification due to the shock compression, and 2) the error introduced when the signal is propagating through the (numerically) viscous region around the shock. This scenario is shown in Fig. 1, where δ denotes the narrow region where the shock-capturing numerics add significant dissipation. The amount of dissipation in this region and its width δ depend on the shock-capturing method and, possibly, the Mach number of the shock. However, for all methods, $\delta \sim h$. Within this idealization, it is clear that the error in the postshock variance is second-order in the grid spacing: loosely speaking, the signal encounters a viscosity $\nu \propto h$ during a time $t \propto \delta \sim h$, which implies that the signal is damped by a factor $\propto h^2$. One purpose of this Note is to verify this view of the shock-capturing error. One simple error metric is the error in the postshock Reynolds stresses $R_{ij} = \widetilde{u_i'' u_j''}$, where $\tilde{}$ denotes a density-weighted (Favre) average, and the double prime $''$ denotes fluctuation around this average. The relative error in R_{ij} is defined as

$$\epsilon_{ij} = \frac{R_{ij}|_{h=0} - R_{ij}|_h}{R_{ij}|_{h=0}} \tag{1}$$

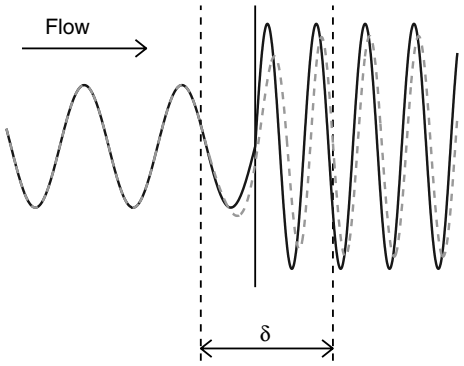

Fig. 1 Sketch of idealized error mechanism in shock-capturing schemes. The solid line shows an incoming signal being modified by the infinitesimal shock (thin solid line) to a higher amplitude and shorter wavelength. The dashed line shows a signal affected by the shock-capturing dissipation (and dispersion) within the numerical shock thickness (δ), leading to both amplitude and phase errors behind the shock.

where subscript $h = 0$ implies the exact or converged value of the average. The purpose of the following is to develop a simple model that predicts this error.

We first assume that the upstream turbulence is isotropic with zero density fluctuations, with a velocity field that satisfies the von Karman spectrum [3]:

$$E(k) = 1.1185 \frac{u^2}{k_0} \frac{(k/k_0)^2}{[(k/k_0)^2 + 5/6]^{11/6}} \tag{2}$$

where the spectrum has been written in a form that gives peak energy at wave number k_0. To approximate LES, the spectrum is truncated at the cutoff wave number $k_{\max} = \pi/h$.

To get an expression for the error in the postshock statistics, we need to approximate both the inviscid compression of the turbulence and the damping due to numerical dissipation. A simple approach is to use homogeneous RDT, where the velocity fluctuations are assumed to be solenoidal. The most obvious flaw in this type of RDT is the assumption of homogeneity, which is incorrect at the shock; a second flaw is that it neglects the generation of acoustic and entropy waves during the interaction (cf., Jacquin et al. [4]).

Decomposing the velocity as $u_i = U_i + u_i'$, the mean compression is taken as $\partial_1 U_1 = -S$ and $\partial_j U_i = 0$ for $(i, j) \neq (1, 1)$. With the assumption of solenoidal turbulence u_i', the RDT system becomes (cf., Pope [3])

$$\partial_t \rho = S\rho; \qquad \partial_t u_i' = -U_1 \partial_1 u_i' + S u_1' \delta_{i1} - \frac{\partial_i p'}{\rho} + \nu \partial_{jj}^2 u_i'$$

where the viscous term in the Navier–Stokes equations has been kept for later use in modeling the shock-capturing dissipation. Following Pope [3], this system is solved using a time-dependent wave number k_1 that satisfies $\partial_t k_1 = S k_1$. We also introduce the normalized time $\tau = St/\ell_n(r)$, where $r = \rho_d/\rho_u$ is the compression ratio of the shock. This yields

$$\frac{\mathrm{d}\hat{u}_i}{\mathrm{d}\tau} = \ell_n(r) \left[\left(\delta_{i1} - 2\frac{k_1 k_i}{k^2} \right) \hat{u}_1 - \frac{\nu k^2}{S} \hat{u}_i \right] \tag{3a}$$

$$k_1 = k_{1,u} r^\tau \tag{3b}$$

which is to be integrated from $\tau = 0$ to 1.

We now seek to model the effect of the numerical shock-capturing dissipation in this framework. Any shock-capturing method necessarily reduces to first order at the shock; therefore, the numerical viscosity should scale as $\nu \sim \Delta U_1 h \sim S h^2$. Since shock-capturing methods tend to capture shocks over a constant number of grid points, one might expect $\nu \approx C S h^2$ for some constant C that should depend on the numerical method but not on the shock compression ratio.

This expression for ν could be inserted into Eq. (3a) directly, but this is not done here. The main flaw of RDT is the assumption of homogeneity. Observations from numerical experiments suggest that most of the numerical dissipation occurs on the downstream side of the smeared shock. This is plausible for two reasons:

1) The shock compresses the turbulence to higher wave numbers (that are more affected by dissipation).

2) The downstream convection velocity is lower, implying that the turbulence spends more time within the numerical shock thickness δ on the downstream side.

This effect can be approximately accounted for in the homogeneous RDT by modeling the full viscous term as

$$\frac{\nu k^2}{S} \hat{u}_i \approx C h^2 k_d^2 \hat{u}_i$$

That is, by replacing (in the viscous term only) the time-dependent wave number $k^2 = k_j k_j$ by its downstream value $k_d^2 = k_{1,u}^2 r^2 + k_2^2 + k_3^2$. With this modeled shock-capturing dissipation, the final RDT model of the numerical shock/turbulence interaction becomes

$$\frac{\mathrm{d}\hat{u}_i}{\mathrm{d}\tau} = \ell_n(r) \left[\left(\delta_{i1} - \frac{2\kappa_1 \kappa_i}{\kappa^2} \right) \hat{u}_1 - C k_0^2 h^2 \kappa_d^2 \hat{u}_i \right]; \qquad \kappa_1 = \kappa_{1,u} r^\tau \tag{4}$$

where the nondimensional wave number $\kappa_i = k_i/k_0$ has been introduced, with k_0 being a characteristic wave number of the upstream turbulence. It is taken as the wave number of peak energy in the present study, but it could also be taken to correspond to the integral length scale or similar.

The RDT model in Eq. (4) is a function of the shock compression ratio r, the nondimensional grid spacing $k_0 h$, and the upstream energy spectrum $E(k)$ (through the initial condition). The constant C in the expression for the implied numerical dissipation is unknown and depends on the numerical method. For 3-D initial conditions, the RDT model can be solved numerically using any ordinary-differential-equation solver, but an analytical solution is possible for single-mode disturbances.

Analytical Solutions for Single-Mode Disturbances

We consider two idealized cases where the incoming disturbance consists of a single mode. When coupled with a numerical experiment, the analytical solution allows for the constant C to be determined. In addition, the analysis illuminates some features of the error introduced by the shock capturing.

Consider first the single-mode disturbance given by $k_{1,u} = k_0$, $\hat{u}_{2,u} \neq 0$, and k_2, k_3, $\hat{u}_1$, and $\hat{u}_3$ all zero (i.e., a disturbance in the transverse velocity component). The RDT model in Eq. (4) for this case becomes

$$\frac{\mathrm{d}\hat{u}_2}{\mathrm{d}\tau} = -C\, \ell_n(r) k_0^2 h^2 r^2 \hat{u}_2$$

which can be solved analytically. Inserting the solution into the error definition in Eq. (1) and expanding the exponential yields the predicted error as

$$\epsilon_{22,\text{single-mode}} \approx 2C\, \ell_n(r) r^2 k_0^2 h^2 \tag{5}$$

Next, consider a disturbance in the shock-normal velocity component (i.e., with $k_2 = k_0$, $\hat{u}_{1,u} \neq 0$, and k_1, k_3, $\hat{u}_2$, $\hat{u}_3$ all zero). Again, solving the RDT model analytically and inserting into the error definition yields the predicted error as

$$\epsilon_{11,\text{single-mode}} \approx 2C\, \ell_n(r) k_0^2 h^2 \tag{6}$$

For both transverse and normal disturbances, the RDT model predicts that the error is second-order in the grid spacing. This is consistent with the simple arguments given previously. Interestingly, the model predicts different error scalings with the strength of the shock r, with the error in the normal and transverse components

scaling as $\ell_n(r)$ and $\ell_n(r)r^2$, respectively. The factor r^2 makes intuitive sense, since this corresponds to the increase in the shock-normal wave number during the interaction with the shock. The RDT model assumes solenoidal turbulence, thus zero streamwise wave number for the normal velocity disturbances; hence, the factor r^2 is absent in $\epsilon_{11,\text{single-mode}}$.

Numerical Experiment: Single-Mode Transverse Disturbance

A first verification of the predictions of the error model is done by computing a numerical experiment of a single-mode interaction. This is only done for the transverse incoming disturbance. The numerical experiment is set up with a stationary shock, and the postshock Reynolds stress is calculated by averaging over several periods in time. A range of mean Mach numbers is chosen to yield density jumps of $r = 1.5$, 2.5, 3.5, 4.5, and 5.5. With gas constant $\gamma = 1.4$, this implies Mach numbers of 1.29, 1.89, 2.65, 3.87, and 7.42. At the inlet, the transverse velocity is set to $u_{2,u} = 0.01\tilde{u}_{1,u}\cos(k_0\tilde{u}_{1,u}t)$ (i.e., a disturbance with wave number k_0 and 1% amplitude). The shock is located one wavelength from the inlet, and a sponge region is used to damp the solution before reaching the outlet boundary. The experiment is run using weighted essentially nonoscillatory (WENO) schemes of third-, fifth-, and seventh-order accuracy with Roe flux splitting. The computed errors are shown in Fig. 2. Also shown are the predicted error scalings from Eq. (5), with C chosen to best fit the results. The results show several things. First, the error is second-order in the grid spacing, as expected. Second, the errors from the different Mach numbers collapse onto a single curve. Given the large range in Mach numbers, this suggests that the RDT model correctly predicts this effect. Finally, as expected, the effect of the numerical method shows up in the constant C. A fit to the numerical results yields

$$C = \begin{cases} 0.090 & \text{third-order WENO} \\ 0.050 & \text{fifth-order WENO} \\ 0.035 & \text{seventh-order WENO} \end{cases}$$

Numerical Experiment: Broadband Isotropic Turbulence

The next numerical experiment is the interaction between isotropic turbulence and a normal shock wave. The method by Ristorcelli and Blaisdell [5] is used to generate isotropic turbulence with peak energy at wave number $k_0 = 4$, which is then allowed to decay in a periodic box of size $(2\pi)^3$ until it becomes fully developed. This developed turbulence is fed into the domain, where it interacts with a normal shock. Immediately upstream of the shock, the Reynolds number based on the Taylor scale [3] is $Re_\lambda \approx 200$, and the mean and turbulent Mach numbers are 1.87 and 0.16, respectively. The transverse grid spacing $h_{2,3}$ is held constant for all cases at $k_0 h_{2,3} = 2\pi/16$, or 16 points per wavelength of the most energetic mode. This is representative of LES, and it is much coarser than that required to resolve the viscous dissipation. The simulations are run without any subgrid model to truly represent underresolved LES and to remove the (basically unknown) behavior of the subgrid model at the shock as a source of uncertainty. To minimize numerical dissipation, a sixth-order-accurate central difference scheme is used away from the shock, whereas the fifth-order WENO scheme is used around the shock [2]. Figure 3 shows a sample of the convergence process. Note that the width of the averaged shock is entirely set by the unsteady shock wrinkling; the instantaneous shock profiles are much steeper. It is clear that the turbulence is damped in the shock region by the numerical dissipation and that this yields significant errors in the postshock Reynolds stress. For this case, a shock-normal grid spacing that is about 16 times finer than the transverse grid spacing is required to bring the error in the postshock transverse Reynolds stress below 1%. Note that the turbulence away from the shock is overly resolved in the shock-normal direction; therefore, the shock-normal grid refinement primarily affects the error generated at the shock. Also note that the turbulence is severely underresolved in the transverse directions behind the shock, which makes the downstream turbulence development unrealistic [2]. For this reason, the error in the postshock Reynolds stresses, as defined by Eq. (1), is computed near the shock at $k_0 x_1 = 0.8$. This error is shown in Fig. 4, along with the predicted error from the RDT model. It is clear that the errors in both the shock-normal and transverse components are second-order in the grid spacing h_1 for sufficiently fine grids. Hence, the idealized picture of the shock-capturing error given previously is valid, even with broadband 3-D turbulence. In contrast with the single-mode experiment, the errors with broadband 3-D turbulence are much larger than predicted by the RDT model, especially in the shock-normal Reynolds stress. The reason for this discrepancy is that

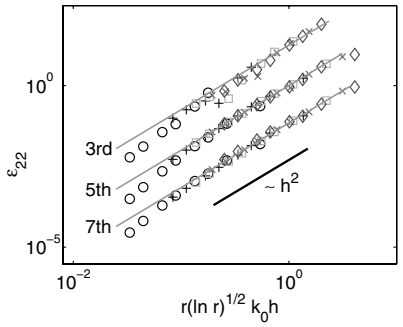

Fig. 2 Error in Reynolds stress from numerical experiment of transverse single-mode disturbance at five different Mach numbers corresponding to density jumps r of 1.5 (circles), 2.5 (plus signs), 3.5 (squares), 4.5 (crosses), and 5.5 (diamonds). The predicted error from Eq. (5) is shown in solid lines, with the constant C chosen to best fit the results. Results from seventh-order WENO ($C = 0.035$), fifth-order WENO ($C = 0.050$, offset by a factor of 10), and third-order WENO ($C = 0.090$, offset by a factor of 100).

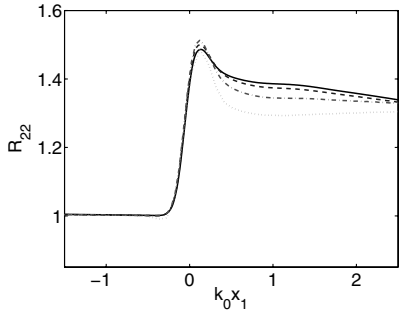

Fig. 3 Convergence of transverse Reynolds stress $R_{22} = \widetilde{u_2''u_2''}$ as the shock-normal grid spacing h_1 is refined, with k_0h_1 of $2\pi/512$ (solid line), $2\pi/256$ (dashed line), $2\pi/128$ (dash-dotted line), and $2\pi/64$ (dotted line). The transverse grid spacing is $k_0h_{2,3} = 2\pi/16$. The Reynolds stress is normalized by its value immediately upstream of the shock.

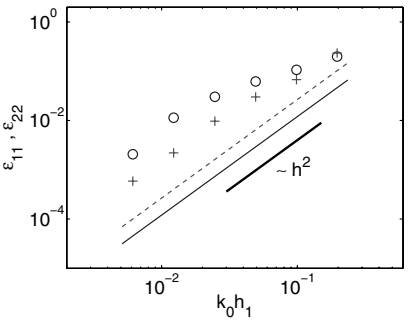

Fig. 4 Error in the postshock Reynolds stresses from numerical experiment of isotropic turbulence at Mach 1.87 with underresolved LES-like grid (symbols) compared with the predicted error from the RDT model (lines). Shock-normal component ϵ_{11} (circles and solid line) and transverse component ϵ_{22} (plus signs and dashed line).

the RDT model fails to take into account both the unsteady shock motion (which affects the amplification ratios) and the generation of sound waves by the shock/turbulence interaction (which primarily affects the shock-normal velocity field). Nevertheless, the RDT model gives the correct scaling of the error and is, therefore, a useful tool for designing grids that minimize the error induced by the shock-capturing dissipation.

Conclusions

It is argued and verified that the error in the postshock Reynolds stresses is second-order, not first-order, in the shock-normal grid spacing when a shock-capturing numerical scheme is used. While not shown, this also holds for several other statistics (e.g., vorticity variances). An error model based on RDT is proposed in the spirit of having a model that is simple yet applicable to broadband 3-D turbulence. The RDT model is shown to correctly predict the error scaling in both single-mode and broadband numerical experiments and to correctly predict how the error scales with shock strength in the single-mode example; however, the model underpredicts the error in the broadband turbulence. Let us consider the implications for DNS and LES separately.

The DNS calculations by Larsson and Lele [2] used grids with $k_0 h_{2,3} = 2\pi/96$ in the transverse directions and refined by factors between two and three (i.e., $k_0 h_1 \lesssim 0.033$) in the shock-normal direction near the shock in order to capture the unidirectionally compressed turbulent structures in that region. Since this was DNS, the energy spectrum of the incoming turbulence decayed rapidly at higher wave numbers. Applying the RDT model to the actual spectrum in the DNS [rather than Eq. (2)] yields the predicted errors $\epsilon_{11} \approx 0.9(k_0 h)^2$ and $\epsilon_{22} \approx 1.7(k_0 h)^2$. This implies errors of less than 0.2% on the DNS grids; therefore; the error induced at the shock was not dominant in these calculations. At higher Reynolds numbers, on finer grids, this will be even more true.

The story is different in LES. The RDT model (with the truncated von Karman spectrum) predicts $\epsilon_{22} \approx 2.6(k_0 h)^2$ for the broadband turbulence example presented here. This implies that $k_0 h \lesssim 0.062$ is needed for 1% error or, equivalently, $k_{\max}/k_0 = \pi/(k_0 h) \gtrsim 50$. The transverse grid resolution in LES should be such that $k_{\max}$ is in the early inertial subrange, say $k_{\max}/k_0 \approx 8$ or so (this corresponds to using a 64^3 grid for isotropic turbulence, with $k_0 = 4$). Hence, the grid must be refined by a factor of six in the shock-normal direction to minimize the error at the shock. If the underprediction of the error by the RDT model in the example presented here is taken into account, an additional factor of two to three is needed. This is a very severe restriction on the required grid.

Is such a strict requirement necessary in practice? The damping occurs primarily at the smallest resolved scales, so these will be underpredicted on the downstream side of the shock. If the subgrid model compensates appropriately, either by introducing energy at those scales (backscatter) or by decreasing the energy transfer for some distance behind the shock, then it is possible that the overall LES results will still be accurate, even in the presence of significant errors at the shock. Therefore, the present work suggests that there is a need to investigate how LES subgrid models behave at and behind a shock, and that the numerical damping at the shock should be taken into account in such studies. Since different numerics introduce different amounts of damping, it is also clear that any given subgrid model should be tested with different numerical methods for a thorough evaluation.

Finally, we mention the possibility of using the error predictions developed here in grid adaptation algorithms (presumably for unstructured grids). In that case, the predicted error could be used to determine the size and shape of the adapted grid cells near shocks.

Acknowledgments

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