Shock-turbulence interaction: What we know and what we can learn from peta-scale simulations

Sanjiva K. Lele1 and Johan Larsson2
1Professor, Dept. of Aeronautics & Astronautics, Durand Building, Stanford University, Stanford, CA 94305-4035
2Research Associate, Center for Turbulence Research, Stanford University, Stanford, CA 94305-3035
E-mail: lele@stanford.edu

Abstract. Many applications in engineering and physical sciences involve turbulent flows interacting with shock waves. High-speed flows around aerodynamic bodies and through propulsion systems for high-speed flight abound with interactions of shear driven turbulence with complex shock waves. Supernova explosions and implosion of a cryogenic fuel pellet for inertial confinement fusion also involve the interaction of shockwaves with turbulence and strong density variations. Numerical simulations of such physical phenomena impose conflicting demands on the numerical algorithms. Capturing broadband spatial and temporal variations in a turbulent flow suggests the use of high-bandwidth schemes with minimal dissipation and dispersion, while capturing the flow discontinuity at a shock wave requires numerical dissipation.

Results from three promising shock-capturing schemes a) high order WENO, b) nonlinear artificial diffusivity with compact finite differences, and c) a hybrid approach combining high-order central differencing with WENO near the shocks are compared using the Taylor-Green problem and compressible isotropic turbulence with eddy-shocklets. The performance of each scheme is characterized in terms of an effective bandwidth. The comparison highlights the damaging effect of numerical dissipation when the WENO scheme is applied everywhere. The hybrid approach is found to be best suited for studying shock-turbulence interactions.

Results from previous DNS and LES studies of the canonical shock-turbulence interaction problem, i.e. the interaction of isotropic turbulence with a (nominally) normal shock and comparison with available theory and experimental data are recalled. The principal physical effects include the amplification of turbulent kinetic energy across the shock and its anisotropy, change in turbulence length scales across the shock, departure from the common assumption of strong Reynolds analogy (used in modeling turbulence in high-speed flows), and the distortion of the shock due to its interaction with the incident turbulence. In this context new results from our SciDAC sponsored project are shown and open issues are mentioned. New DNS results achieve a significantly larger turbulence Reynolds number and allow an exploration of the nonlinear effects. While the linear interaction theory of Ribner provides useful estimates of the amplification of vorticity fluctuations across the shock, it misses the strong nonlinear dynamics of the energized and highly anisotropic vorticity downstream of the shock. It is found that previous DNS studies also underestimated this effect. The simulations show that turbulent self-stretching and tilting mechanisms bring about a relatively rapid return to isotropy in the turbulent vorticity field. The turbulent velocity field, however, does not show any appreciable tendency towards isotropy. It is further observed that when the turbulence interacting with the shock is sufficiently energetic the instantaneous shock structure is significantly modified; local regions of significant over-compression are found as well as regions where the mean shock compression is nearly isentropic. Estimates for the computational resources necessary for studying this fundamental shock-turbulence interaction problem at higher Reynolds number on peta-scale computing systems are given.
**1. Introduction**

Most fluid flows of scientific and engineering interest involve and are strongly affected by turbulence. For example, turbulence has a great effect on the process of mixing, which in turn has a major effect on flow separation, combustion, and other phenomena. When interacting with a shock wave, the state of turbulence changes dramatically. Thus it is clear that the interaction of turbulence with a shock wave is a key feature in many high-speed engineering systems. The most fundamental problem in this area is that of isotropic turbulence passing through a nominally normal shock. This idealized problem allows a study of the mechanics of the mutual interaction between the turbulence and the shock wave without the complications which arise from the boundary layer separation and the attendant low frequency unsteadiness (cf. Dolling [1] and Dupont *et al.* [2] for discussions of the shock wave turbulent boundary layer interaction).

This canonical problem shown in figure 1 has received considerable attention in past theoretical [3], experimental [4, 5], and computational [6–8] studies. The linear theory by Ribner [3] predicts that the velocity and vorticity variances are amplified during the shock interaction, and that there is an inviscid adjustment region behind the shock where the evanescent acoustic modes and turbulence adjusts to establish the post-shock state. This theory is formally valid in the limits of infinite Reynolds number and zero turbulent Mach number, but has thus far [6–8] only been tested at Reynolds numbers of $Re_\lambda \approx 20$. At these low Reynolds numbers, the viscous decay behind the shock is comparable to or larger than the inviscid adjustment, which makes direct comparisons to the linear theory difficult. Furthermore, the spectrum of turbulence is not truly broadband at such Reynolds numbers. The objective of the present study is to use direct numerical simulation (DNS) to produce a set of highly resolved databases at higher Reynolds number, to be used in examination of the validity of the linear theory as well as in *a priori* and *a posteriori* studies of modeling shock/turbulence interaction in the context of large eddy simulation (LES) and engineering turbulence closures.

**2. Numerical method assessment for shock-turbulence interaction**

A collaborative assessment of several numerical approaches to shock capturing on a suite of benchmark test problems deemed relevant for studying the interaction of shocks with turbulence was undertaken by our SciDAC project team. A comprehensive discussion of the test problems,
algorithms, and detailed results are given in Ref. [9]. A short summary is included here for completeness. Results from three approaches are compared in this paper.

2.1. WENO
Weighted essentially non-oscillatory (WENO) schemes are generally considered to be state-of-the-art for shock-capturing. Here we include a standard 7th-order WENO method with Roe flux-splitting [10].

2.2. Nonlinear artificial viscosity
The nonlinear artificial viscosity/hyperviscosity approach originally proposed by Cook and Cabot [11] and further refined by Cook [12] is used. It essentially consists of adding artificial (or numerical) viscosities, diffusivities, and conductivities to the physical properties that are designed to smooth out discontinuities sufficiently such that they can be captured by a high-order central difference scheme, to mimic the energy transfer to unresolved small scales (i.e., function as a subgrid scale model in the context of large-eddy simulation), and to vanish in well resolved regions of the flow. These artificial properties take the form of high order derivatives of the resolved velocity field, thus become large around discontinuities and small elsewhere. The augmented governing equations are integrated using high-order compact finite differences. To maintain stability and minimize aliasing errors, the solution is filtered after each time step using a compact filter biased towards the smallest scales. Results shown in this paper were obtained using an in-house code by A. Bhagatwala which has very good resolution properties [13]. While the method was originally intended to always include all different artificial fluid properties, we consider two different permutations here: a minimally dissipative method with only the artificial bulk viscosity and the compact filter (the minimal requirements for capturing shock waves), and the same with added shear-viscosity (closer to the original [11, 12] model).

2.3. Hybrid approach
The hybrid method is based on the idea that broadband turbulence and discontinuities represent different physics and thus should be treated by different numerical methods. It consists of essentially three components that can be chosen rather freely: a central finite-difference scheme for the smooth regions, a shock-capturing scheme for the regions containing discontinuities, and a solution-adaptive sensor which identifies these regions. For shock-capturing, a 5th-order WENO method [10] is chosen due to its ability to capture shocks in a sharp fashion with few adjustable parameters. Away from the shocks, an 6th-order central difference scheme is used on a split form of the convective terms that improves nonlinear stability. These schemes are coupled in a conservative manner that preserves stability [14]. The shock sensor is inspired by the observation that shock waves are associated with large negative dilatation, whereas turbulence is associated with large vorticity. Comparing these quantities then yields an effective shock sensor. The primary advantage of the hybrid approach, as compared to a ‘shock-capturing only’ method, is that numerical dissipation is restricted to the regions flagged by the sensor, which will be shown to drastically improve predictions of turbulence spectra.

3. Effective bandwidth on nonlinear problems
Results from the Taylor-Green problem and from compressible isotropic turbulence are used to characterize the range of well-resolved scales or effective bandwidth of the algorithms being used. The effective bandwidth is quantified by comparing the results to those obtained from a reference calculation using much higher resolution; it was shown in Ref. [15] that the reference calculations are of sufficiently high quality to be useful as a benchmark. The effective bandwidth is defined as the wavenumber range over which the computed energy spectrum is within a specified tolerance.
from the ‘reference energy spectrum’ obtained in the reference calculation. The tolerance is set to be a deviation of ±25% from the reference spectrum.

3.1. Taylor-Green results

Figure 2 shows the evolution of kinetic energy and enstrophy for the Taylor-Green problem. For this inviscid problem there is no viscous dissipation and the kinetic energy should remain the same as its initial value. However beyond the non-dimensional time of 3 units there is a rapid build-up of fine-scale structures in the flow due to vortex-stretching and tilting, and numerical schemes begin to dissipate the kinetic energy at various rates. The hybrid scheme is exceptional in that it conserves kinetic energy exactly and maintains this property even for severely under-resolved flow features. Consequently the enstrophy growth predicted by the hybrid scheme is the highest amongst the methods used.

The effective bandwidth of the various schemes can be judged from figure 3 where compensated kinetic energy spectra, i.e. $E(k)/E_{\text{ref}}(k)$, are plotted at $t = 5$ (after the small-scale growth). The lines corresponding to ±25% deviation are also shown. The effective bandwidth for WENO is only about 1/4 of the wavenumber range which can be represented on mesh used. The non-dissipative methods (hybrid and compact) are accurate up to almost 2/3 of the wavenumber range, while the different forms of added dissipation lowers this to about 1/2.

3.2. Compressible turbulence with eddy shocklets

A more stringent test case is that of decaying isotropic turbulence at high turbulent Mach number $M_t$. The turbulence spontaneously generates eddy shocklets which activate the various shock-capturing numerics and excessive numerical dissipation can lead to dramatic errors. We first compute a well-resolved DNS on a $256^3$ grid at initial $M_t = 0.6$ and microscale Reynolds number $Re_\lambda = 100$. On this grid all methods converge to the same solution.

We then assess the different algorithms by comparing results obtained on a $64^3$ grid. The decay of turbulent kinetic energy (TKE) with time is not sufficiently sensitive to judge the difference between the various schemes used here [15]; it is thus not shown here. Figure 3 shows the effective bandwidths obtained in the simulation of this nonlinear compressible turbulence
Figure 3. Compensated kinetic energy spectrum (at $t = 5$ on left panel for Taylor Green problem and at $t = 4$ (right panel) for compressible isotropic turbulence) on 64$^3$ grids. Different curves correspond to different algorithms. Solid black: converged reference; solid blue: hybrid method; solid red: optimized compact scheme; dashed red: optimized compact scheme with shear-viscosity; dashed blue: hybrid with 8th order dissipation; dotted blue: hybrid with dynamic Smagorinsky model; green: WENO.

These results are consistent with the trends noted earlier for the Taylor-Green problem. The WENO scheme is accurate over only $1/4$ of the wavenumber range. The compact scheme with artificial viscosity and hybrid scheme with high-order dissipation or dynamic SGS model all capture approximately $1/2$ of the wavenumber range accurately. Only the minimally dissipative schemes capture $2/3$ of the wavenumber range.

These results characterize the performance of various shock-capturing schemes on compressible turbulence problems in a fundamental way. Assessment of several additional numerical schemes was included in our collaborative work under the SciDAC project. These tests also included test cases emphasizing shock capturing ability for strong shocks, and interactions with density interfaces. A comprehensive report on these comparisons is available through the project website (see http://shocks.stanford.edu).

4. Canonical shock/turbulence interaction

The most fundamental shock/turbulence interaction problem is that of isotropic turbulence passing through a nominally normal shock wave (or, equivalently, a normal shock passing through isotropic turbulence). The essence of the problem is shown in figure 1. The incoming turbulence is isotropic, as evidenced by the random orientation of the vortex cores. The shock compresses the turbulence in the $x$ direction, increasing the vorticity and making the post-shock turbulence axisymmetric with vortex cores predominantly oriented in the $y-z$ plane. Ribner [16] studied the problem analytically by solving the linearized Euler equations with linearized shock jump conditions for incoming purely vortical turbulence. This linear interaction analysis (LIA) assumes that the turbulence comprises a small perturbation relative to the shock and that nonlinear effects in the post-shock evolution are small (as well as the standard assumption of a difference in time scales). In addition, the Rankine-Hugoniot shock jump conditions are incorporated into LIA; one consequence is that LIA captures the generation of sound and entropy waves from incoming purely vortical turbulence.

Lee et al. performed a set of landmark direct numerical simulations (DNS) of canonical shock/turbulence interaction in a sequence of papers [6, 7]. The first of these papers considered shocks at Mach numbers up to 1.2 where the viscous structure of the shock was resolved; these
were therefore truly direct solutions of the Navier-Stokes equations. In the second paper they verified that these “true” DNS results at Mach 1.2 could be replicated by instead capturing the shock (at considerably lower cost), provided sufficient grid resolution in the shock-normal direction at the shock. This methodology was then used to compute cases at Mach numbers up to 3. When comparing the results to LIA predictions, they found that LIA realistically represents many features, including the amplification of transverse vorticity, the amplification and post-shock evolution of the Reynolds stresses, and the decrease in transverse Taylor length scale. Mahesh et al. [8] considered the influence of entropy fluctuations in the upstream turbulence, and found that negatively correlated velocity and temperature fluctuations lead to enhanced amplifications of turbulence kinetic energy and vorticity. Later, Jamme et al. [17] resolved the viscous shock structure at Mach 1.2 and 1.5, and essentially confirmed the findings of Mahesh et al. Barre et al. [5] studied the problem experimentally in a wind tunnel, and measured velocity variances using hot-wires and LDV.

The present study builds on these previous studies, especially those by Lee et al. [6, 7]. In this paper, DNS in the extended sense of capturing the shock while directly resolving all scales of turbulence is used. Highlights of the new DNS results are shown in this paper, with a more detailed account available in Larsson and Lele [18]. It is shown that a simple argument about the Kolmogorov scale implies that DNS requires a refined grid in both the shock-normal and the transverse directions to fully resolve the viscous scales of turbulence. This is verified by a grid convergence study, and implies that the calculations in the studies mentioned above were, most likely, under-resolved. The present DNS data is fully resolved, which leads to larger differences between the data and LIA. The Reynolds stresses are more anisotropic in the present DNS, and there are qualitative differences in the Taylor length scales. Moreover, the vorticity components return to isotropy in all cases in the present study. This raises the interesting question of whether under-resolution of the post-shock turbulence in previous DNS essentially neglects some phenomenon that is also neglected in the LIA. This will be explored below.

Throughout this paper the subscripts “u” and “d” refer to average states upstream and downstream of the shock, respectively. For quantities that evolve in the streamwise direction, these states are obtained by extrapolation to the average shock location. The mean flow and turbulent Mach numbers are defined as $M = \frac{u_1}{c}$ and $M_t = \sqrt{\langle u_i' u_i' \rangle / c}$, respectively, where $u_1$ is the streamwise velocity and $c$ is the speed of sound. To minimize errors around the shock, a stretched grid is used in the streamwise direction with finer mesh spacing in the vicinity of the shock. The inflow turbulence is taken from a pre-computed database of isotropic turbulence. At the outflow, a sponge region is used to gently drive the flow toward a laminar state.

4.1. Grid resolution requirements
The most severe resolution requirement for DNS of shock-turbulence interaction come from the need to resolve the dissipative scale motions in the post-shock turbulence. In addition, since the vorticity field in the post-shock turbulence rapidly becomes isotropic, a finer grid in the post-shock region is needed in all directions. Larsson and Lele [18] estimated the post-shock Kolmogorov scale using rapid-distortion theory scaling. Comparison of this estimate with DNS data is shown in figure 4. They also conducted grid refinement studies for several shock-turbulence interactions using successively refined grids. At the relatively modest turbulence microscale Reynolds number $Re_\lambda = 40$, a grid with $1040 \times 384^2 \approx 153 \times 10^6$ grid points was found to be necessary to ensure that the estimated error in the velocity and vorticity variances was less than 2%.

4.2. Turbulence amplification and anisotropy
The variances of velocity and vorticity fluctuations are shown in figure 5 for a sequence of cases. The transverse vorticity is directly amplified at the shock due to the compression, while the
Figure 4. Left: Change in the Kolmogorov scale across the shock as a function of Mach number. Estimate from Ref. [18] in lines with $\gamma = 1.4$ (solid blue) and $\gamma = 5/3$ (dashed red). Results from DNS in symbols. Right: Mean density profiles for mean Mach number $M$ of 1.5 (dashed lines) and 1.9 (solid lines), with turbulent Mach number $M_t$ of 0.22 (blue) and 0.31 (red). The inviscid Rankine-Hugoniot jumps are shown in dotted black lines. Note that the mean pressure profiles are similar.

Figure 5. Canonical shock/turbulence interaction on $1040 \times 384^2$ grid. Left: variance of Reynolds stress ($\langle u'u' \rangle$ in solid lines, $\langle v'v' \rangle$ in dashed lines). Right: variance of vorticity ($\langle \omega_1 \omega_1 \rangle$ in solid lines, $\langle \omega_2 \omega_2 \rangle$ in dashed lines). Mean Mach number $M$ of 1.9 (blue) and 3.5 (red).

Streamwise vorticity is initially unchanged. Behind the shock, the out-of-equilibrium turbulence adjusts towards an isotropic state, although the Reynolds stresses never reach isotropy in these runs. One outstanding question in shock/turbulence interaction is whether the turbulence truly returns to isotropy. The low Reynolds number of the present (and all previous) runs implies a quick viscous decay behind the shock, which overwhelms any return-to-isotropy. Large-scale calculations at higher Reynolds numbers are needed to illuminate this issue.

4.3. Mean fields
The coupling between the changes in the turbulence and the mean flow can be illustrated by the profiles of mean density across the shock. Figure 4 shows such profiles for a sequence of simulations at different shock Mach number $M$ and turbulence Mach number $M_t$. Note that for a fixed low value of $M_t = 0.15$ as $M$ is increased the mean profiles show the expected tendency...
following the standard Rankine-Hugoniot jump conditions. However, when we consider the changes at fixed $M$ but increasing $M_t$, an effect associated with turbulence becomes apparent. Profiles of mean density (and pressure) display a more complex two-stage structure at higher $M_t$; evidently in the immediate vicinity of the shock the mean density rise is smaller than the Rankine-Hugoniot jump, with this deficit recovered in an extended region downstream of the shock. Further study of the change in mean shock structure for sufficiently vigorous incident turbulence is warranted. The present data are qualitatively consistent with an analysis of the turbulent flow shock jumps by Lele [19], who used rapid distortion theory to close the jump conditions.

4.4. Change in shock structure

At high enough turbulent Mach number $M_t$, the turbulent pressure fluctuations in the turbulence upstream of the shock become comparable to the pressure jump associated with the shock, which significantly alters the instantaneous shock structure. A snapshot of a strongly wrinkled instantaneous shock is shown in figure 1. It is clear that the shock is not simply planar at high $M_t$, but instead a rather complex object. The small “holes” in the shock are regions of nearly isentropic smooth compression. Some instantaneous profiles of density and dilatation along the $x$ axis are shown in figure 6 for such a case. The instantaneous structure of the shock varies wildly, from being twice as strong as on average (note the significant over-compression and subsequent recovery) to being replaced by a relatively smooth compression wave. This intermittency is largely absent at lower values of $M_t$, and represents an outstanding fundamental question in shock/turbulence interaction. It is expected that at higher Reynolds number such intermittency may be quite strong and substantially affect the change across the shock wave.

4.5. Effect of numerical dissipation in shock-turbulence simulations

In a previous section we noted the effect of numerical dissipation in the context of the Taylor-Green and compressible isotropic turbulence problems. The 7th order WENO scheme provided an accurate representation of the energy spectrum in these flows only for 1/4 of the resolvable wavenumber range, i.e., significant dissipation was observed over the upper 3/4 range of wavenumbers. We now demonstrate the serious effect of numerical dissipation in the canonical shock-turbulence interaction problem. Results from the previous section on shock-turbulence simulations ($M = 1.5$ and $M_t = 0.22$) computed with the hybrid code are plotted against results...
Figure 7. Effect of numerical dissipation on shock/turbulence interaction. Converged DNS on $1040 \times 384^2$ grid (black), 5th-order hybrid scheme on $347 \times 128^2$ grid (blue), and 7th-order WENO scheme on $347 \times 128^2$ grid (red). Left: variance of Reynolds stress ($\langle u'v' \rangle$ in solid lines, $\langle v'h' \rangle$ in dashed lines). Right: variance of vorticity ($\langle \omega_1 \omega_1 \rangle$ in solid lines, $\langle \omega_2 \omega_2 \rangle$ in dashed lines). Mean Mach number $M$ of 1.5.

obtained with the 7th order WENO scheme applied everywhere in the flow. Additionally these results are compared with a finer resolution calculation using the hybrid code.

Figure 7 shows the streamwise evolution of the variances of fluctuating velocity and vorticity. The quantities plotted are normalized by the values immediately upstream of the shock allowing a quantitative comparison of the curves. Note that the hybrid results at the ‘coarse’ resolution of $347 \times 128^2$ are consistently close to the higher resolution $1040 \times 384^2$ results which are regarded as converged results. On the other hand the WENO results at $347 \times 128^2$ resolution show significant dissipation. In particular, the transverse component of the fluctuating velocity and all components of vorticity fluctuation show marked attenuation relative to the converged results. The nonlinear stretching/tilting of shock-normal vorticity is almost fully damped in the WENO results. These results suggest that strong caution must be exercised in using dissipative numerical algorithms in shock-turbulence interaction calculations. Even with relatively high-order dissipative schemes (in this case, 7th-order WENO), important turbulence dynamics can be numerically damped.

4.6. Cost estimates for simulation at higher Reynolds number

Well-resolved direct numerical simulation (DNS) requires adequate resolution of the viscous dissipation, which in isotropic turbulence amounts to having the maximum wavenumber $k_{max} = \pi N_y / D \geq 1.5/\eta$, where $N_y$ is the number of points in the transverse directions, $D$ is the transverse domain size, and $\eta$ is the Kolmogorov length scale. Consider turbulence at $M = 2$, $\gamma = 1.4$, and some $Re_\lambda$ immediately upstream of the shock. The shock compression modifies the Kolmogorov scale by about a factor of $\eta_d/\eta_u \approx (\rho_d/\rho_u)^{-1} (T_d/T_u)^{3/8} \approx 0.46$ (using the simple theory presented in Ref. [18]); therefore the critical resolution is downstream of the shock. The upstream isotropic turbulence approximately satisfies $\eta_u \approx 4.15 L Re_\lambda^{-3/2}$, where $L$ is the dissipation length scale. For the spectra used in this study we have $L \approx 1.7D/(-\eta m_0)$, where $m_0$ is the most energetic mode. Putting this together yields the required transverse resolution of $N_y \geq 0.46 m_0 Re_\lambda^{3/2}$. This is a more stringent criterion than used in previous studies (since it accounts for the change in $\eta$ across the shock), but is necessary to adequately resolve the post-shock dissipative motions.

To resolve the compressed post-shock motions (finer grid in $x$) and cover a sufficiently
large streamwise domain, our present calculations use $N_x \approx 3N_y$ points in the streamwise direction. The grid required to compute a case with $Re_\lambda = 100$ and $m_0 = 4$ is therefore about $5520 \times 1840^2 \approx 19 \cdot 10^9$ points. Finally, the present calculations require about $50N_y$ time steps to fully remove the initial transients and compute statistics, so the sample calculation would require about $10^5$ time steps. With the hybrid code this amounts to approximately 50 million core-hours, which shows the extreme cost of properly performed direct numerical simulation of shock/turbulence interaction.

5. Summary and outlook

The progress towards large-scale calculations of the canonical shock/turbulence interaction discussed here is part of a larger effort towards improved computational methods for complex shock/turbulence interaction problems. The canonical shock/turbulence problem described here serves two purposes in this larger effort. First, it is a useful problem for computational efficiency/accuracy assessment and improvement, since it includes all the relevant algorithmic complexities. It was used here to highlight the strong adverse effects of numerical dissipation. Even for a very high order method (7th order WENO) the numerical dissipation overwhelmed the turbulence evolution downstream of the shock. Secondly, the shock/turbulence calculations will produce large databases at different combinations of turbulent and mean flow Mach numbers, at higher Reynolds numbers than previously possible. These databases will be of use both in theoretical developments, e.g. for assessment of the validity of Ribner’s linear theory at higher levels of compressibility, and in model development, e.g. for \emph{a priori} studies or \emph{a posteriori} comparisons in subgrid scale modeling.

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