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Computational issues and algorithm assessment for shock/turbulence interaction problems

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Abstract. The paper provides an overview of the challenges involved in the computation of flows with interactions between turbulence, strong shockwaves, and sharp density interfaces. The prediction and physics of such flows is the focus of an ongoing project in the Scientific Discovery through Advanced Computing (SciDAC) program. While the project is fundamental in nature, there are many important potential applications of scientific and engineering interest ranging from inertial confinement fusion to exploding supernovae. The essential challenges will be discussed, and some representative numerical results that highlight these challenges will be shown. In addition, the overall approach taken in this project will be outlined.

1. Introduction

Most fluid flows of scientific and engineering interest involve and are strongly affected by turbulence. For example, turbulence typically increases the rate of mixing by orders of magnitude, and the accurate prediction of turbulence and its effects is critical in many areas of science and engineering. Similarly, strong shockwaves and density variations play important roles in many fluid flows. The lift and drag of a supersonic airplane, for instance, is largely determined by the shockwaves around the aircraft.

While the understanding and prediction of flows involving any one of these phenomena is a complex and nontrivial matter, the situation becomes even more difficult for flows where strong interactions between turbulence, shockwaves, and density variations occur. Such is the case in many diverse areas of science and engineering, including supernovae explosions, super- and hypersonic propulsion, the implosion of a cryogenic fuel capsule in inertial confinement fusion (ICF), and several other problems. Due to the inherent complexity, both the scientific understanding of and the capability to accurately predict such flows remains limited. The present project aims at improving both of these aspects.

The computational challenge of predicting flows with shock/turbulence/density interactions stems from the fundamentally different physics at play. Shockwaves are exceptionally thin layers where the state of the fluid changes rapidly over a distance on the order of the molecular mean free path, and thus they can essentially be considered as strong discontinuities in the flow field. Many numerical methods that capture such discontiuities have been developed over the past few decades, and they all rely on numerical dissipation to artificially smooth the discontinuity such that it can be resolved on the computational grid. Turbulence, on the other hand, is a chaotic phenomenon with broadband spatial and temporal spectra, and there is much evidence that excessive dissipation has a profound adverse effect on the computed turbulence. An example that illustrates this effects will be shown below. This inherent dilemma of the effects of numerical dissipation is one (of several) main challenges in the prediction of shock/turbulence interactions. Additional challenges include the fact that many shock-capturing schemes are based on one-dimensional decompositions that potentially creates unphysically anisotropic flow fields, the challenge of combinining accuracy, efficiency, and robustness, and the ever-present fact of turbulence being a broadband chaotic phenomenon with a vast range of length scales that need to be resolved.

1.1. Objectives and outline

The work presented here is aimed at improved predictive computational methods for these challenging problems. As a first step towards bringing to light the strengths and limitations of different approaches we consider the comparison of four distinctly different numerical methods on a suite of benchmark problems. This comparison is not considered a ‘competition’ between methods, but rather as a way to illuminate the effects of various conceptual approaches to shock/turbulence interaction prediction.

We will first briefly describe the different approaches considered, and then show some preliminary results that illustrate certain important concepts.

2. Computional approaches

Following here are brief descriptions of the chosen approaches – for detailed information we refer to the respective references.

2.1. Unified hyperviscosity approach

The hyperviscosity approach was originally proposed by Cook and Cabot [1] and later refined [2, 3]. 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 becoming large around discontinuities and small elsewhere. The augmented governing equations are integrated using a 10th order accurate compact central difference scheme together with a 4th order accurate Runge-Kutta scheme in time. To maintain stability and minimize aliasing errors, the solution is filtered after each time step using a compact filter biased towards the smallest scales. The method has been implemented in a parallel code and run on up to 65,536 processors of the BGL supercomputer with excellent scaling.

2.2. Unified filtering approach

The filtering approach has been developed by Sjögreen and Yee (cf. [4] and references therein), and is aimed at decreasing both the computational cost and the numerical dissipation of any given shock-capturing scheme. With a Runge-Kutta scheme in time, the governing equations are integrated during the substeps using a central difference scheme of high order. At the end of the time step, the solution is then filtered by adding the dissipative portion of any shock-capturing scheme, and potentially also a high order linear dissipation term. This minimizes the computational cost by reducing the number of expensive shock-capturing computations in the method (by a factor of the number of stages in the Runge-Kutta scheme). Equally importantly, it also allows for better control of the amount of numerical dissipation introduced. The method has been parallelized and applied to a range of test problems, demonstrating retained accuracy while substantially reducing the computational cost.

2.3. Hybrid approach

The previously mentioned approaches are both 'unified' in the sense that they apply the same method in the full domain. In contrast, hybrid approaches rely on the idea that broadband turbulence and discontinuities represent different physics and thus should be treated by different numerical methods. Hybrid methods thus consist of essentially three components that can be chosen rather freely: a high order difference scheme for the smooth regions, a shock-capturing scheme for the regions containing discontinuities, and a solution adaptive sensor that identifies these regions. Several hybrid methods have been proposed [5, 6] which differ in some or all of these components. The present hybrid method [7] relies on an 8th order accurate central difference scheme for the turbulence regions and a 7th order accurate WENO scheme [8] for shock-capturing. These schemes are coupled (or interfaced) in a conservative manner that preserves stability. The shock sensor is inspired by the observation that shockwaves are associated with large negative dilatation (compression) whereas turbulence is more typically associated with large vorticity. Comparing these quantities then yields an accurate sensor of shockwaves. The main advantage of the hybrid approach is the minimal amount of dissipation that is introduced, which potentially allows for better predictions of turbulence spectra. A second advantage is the lowered computational cost due to the fact that the expensive shock-capturing scheme is used in only small parts of the domain. Among the drawbacks is the increased sensitivity to numerical instabilities (due to the lower dissipation) and the reliance on a shock-sensor to identify all discontinuities.

2.4. Shock-fitting approach

The final approach considered in this study is also the one that most differs from the others. While in the previous three methods the numerical method is designed to capture shockwaves anywhere in the domain, the shock-fitting approach [9] instead views the discontinuity as an internal boundary between two different domains. At this boundary the analytical jump relations are imposed, thus treating the discontinuity in a consistent manner. Preliminary tests show that this approach can yield substantially more accurate results for problems with simple shock structure. The main challenge is in its application to very complex flows with multiple shock-shock interactions.

3. Results

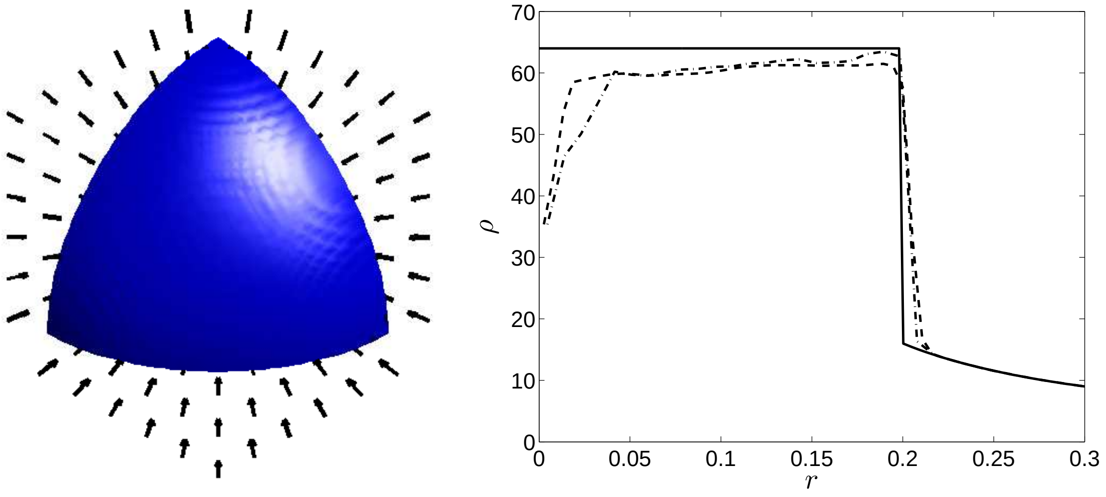
A suite of benchmark problems that assess different attributes of the methods has been identified. Following here are descriptions and some sample results from two of them.

3.1. Spherical implosion

The Noh [10] problem of an infinite Mach number implosion presents a rather severe test of the capability of a shock-capturing method to handle the very strong spherical shockwave that develops. In addition, this problem is a building-block flow for the implosion of a fuel capsule in inertial confinement fusion. The initial condition in Cartesian tensor notation is

$$\rho = 1\,, \quad u_i = -\frac{x_i}{\sqrt{x_1^2 + x_2^2 + x_3^2}}\,, \quad p = 0\,,$$

along with the perfect gas assumption, i.e. an imploding flow towards the origin at infinite Mach number. In response, a strong spherical shockwave develops that is traveling outwards



(a) Contour surface of the shockwave, with vectors indicating the imploding flow.

(b) Density profiles along a grid axis (dashed) and diagonally through the domain (dash-dotted), with analytical solution (solid).

Figure 1. The shockwave generated by a spherical implosion, not unlike that in inertial confinement fusion, computed by a hybrid central/WENO method of 7th order accuracy.

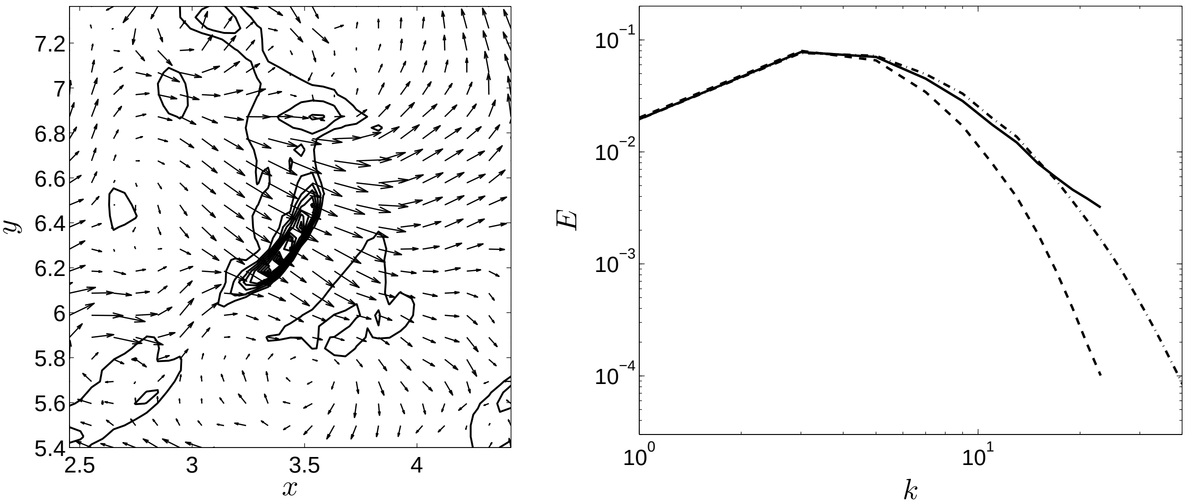
at constant speed. This problem provides an assessment of the capability to predict three key attributes: the post-shock density (i.e., the compression by the shockwave), the correct shock speed, and spherical shape on a Cartesian grid.

Shown in figure 1(a) is one octant of the resulting shockwave front along with the imploding flow computed by the hybrid method briefly described in section 2.3. Despite the Cartesian grid, the shock front is very close to spherical. Profiles of the density are shown in figure 1(b) along and diagonal to the grid. The fact that both profiles essentially agree shows that the grid imprinting errors are small, but there are three other kinds of errors visible: the shock speed is overpredicted, the rate of compression is underpredicted, and there are additional errors near the origin. These errors are all associated with unphysical heating due to the shock-capturing scheme, which the Noh problem is especially sensitive to. The ability to accurately predict very strong shockwaves is essential to the present project, and the Noh problem provides a stringent test of this.

3.2. Isotropic turbulence with shocklets

Isotropic decaying turbulence is a standard test case for high-fidelity numerical methods. The key challenges in this test case are to predict the rate of decay of the important statistical quantities (like kinetic energy) and to predict the correct spectral distribution of energy between the different scales of motion. At high enough Reynolds and Mach numbers, the turbulent motions develop shocklets (weak shockwaves) spontaneously, the capturing of which introduces numerical dissipation which affects the rate of decay and the spectra. Shown in figure 2(a) is a slice through the field at an instant. The chaotic and quasi-random nature of turbulence is evident, as are the local regions of large compression characteristic of shocklets.

To illustrate one core difficulty in the computation of these flows, the spectrum of kinetic energy at an instant is shown in figure 2(b). The hybrid method of section 2.3, which is minimally dissipative due to the use of a central scheme in the majority of the domain, yields a reasonable predicted spectrum up to rather high wavenumbers, whereas the standard 7th order WENO method due to its inherent dissipation produces an underprediction for a large range



(a) Contours of compression and velocity vectors in a plane. The region of high compression in the center signifies a weak shocklet.

(b) Spectra of the kinetic energy after three eddy-turnover times on 48^3 grid. Hybrid method (solid), WENO method (dashed), and reference solution on 256^3 grid (dash-dotted).

Figure 2. Isotropic turbulence with shocklets.

of wavenumbers. This shows that the simultaneous capturing of shockwaves and an accurate prediction of turbulence is challenging, and that methods must be developed with extreme care. That is precisely one core objective of the present project.

4. Summary and future work

The material presented here is part of an ongoing effort towards improved computational methods for complex shock/turbulence interaction problems. There is, therefore, much future work to be done. This includes a detailed comparison of the four computational approaches on the full suite of benchmark problems and, more importantly, to exploit the detailed knowledge generated by this comparison into more accurate, robust, and efficient algorithms.

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