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Summary: This short note discusses some of the challenges for design of suitable spatial numerical schemes for hypersonic turbulent flows, including combustion, and thermal and chemical nonequilibrium flows. Often, hypersonic turbulent flows in re-entry space vehicles and space physics involve mixed steady strong shocks and turbulence with unsteady shocklets. Material mixing in combustion poses additional computational challenges. Proper control of numerical dissipation in numerical methods beyond the standard shock-capturing dissipation at discontinuities is an essential element for accurate and stable simulations of the subject physics. On one hand, the physics of strong steady shocks and unsteady turbulence/shocklet interactions under the nonequilibrium environment is not well understood. On the other hand, standard and newly developed high order accurate (fourth-order or higher) schemes were developed for homogeneous hyperbolic conservation laws and mixed hyperbolic and parabolic partial differential equations (PDEs) (without source terms). The majority of finite rate chemistry and thermal nonequilibrium simulations employ methods for homogeneous time-dependent PDEs with a pointwise evaluation of the source terms. The pointwise evaluation of the source term might not be the best choice for stability, accuracy and minimization of spurious numerics for the overall scheme.

1 Overview

Within the homogeneous time-dependent PDEs, early algorithm development in the pre shock-capturing era concentrated heavily on incompressible flows and low speed compressible flows with weak shocks. For simple geometries, spectral methods [13] have been the method of choice for direct numerical simulations (DNS) and large eddy simulations (LES). For complex geometries, low order central schemes with linear numerical dissipations were used, due to the lack of nonlinearly stable numerical boundary condition treatment for high order central schemes at the time. High order central schemes were advocated by Kreiss & Oliger [21] and Swartz & Wendroff [43] with limited turbulent related application in the pre shock-capturing era. Spatially high order compact schemes (or spatially implicit schemes) initiated by Hirsh [18] and Ciment & Leventhal [6] in the mid 70's were not used for turbulence computation until the work of Lele [25]. Here, high order schemes refer to schemes that are fourth-order or higher away from extrema and discontinuities. For over three decades the spatially second-order or higher MacCormack [29] schemes, Beam and Warming implicit scheme [2] and Steger and Warming flux vector splitting upwind algorithm [41] dominated steady aerodynamic numerical simulations in conjunction with turbulent modeling.

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Since the pioneer shock-capturing work of flux corrected transport (FCT) [3], monotone upwind scheme for conservation laws (MUSCL) [44], piecewise parabolic method (PPM) [7], Roe's approximate Riemann solver [32] and total variation diminishing (TVD) [17] and essentially nonoscillatory (ENO) schemes [19, 36], there has been an explosion of a very wide spectrum of fluid applications during the post shock-capturing era. The main shortcoming of these shock-capturing schemes is the degradation of the overall accuracy of the schemes away from shocks and discontinuities as well as clipping of extrema. Shortly after the introduction of weighted ENO (WENO) by Liu, Osher & Chan [28] in 1994, Jiang and Shu [20] provided a general framework to construct arbitrary order accurate WENO schemes with efficient multi-dimension implementation of their schemes. The main advantage of WENO schemes is their ability to achieve high order accuracy in smooth regions while maintaining stable non-oscillatory discontinuity transitions. For shorter time integrations and/or rapidly developing unsteady complex shock interactions, WENO schemes are now the method of choice for practical convection dominating complex shock interaction applications. For FCT development, see Zalesak [57]. For an overview of basic TVD and ENO schemes, see [45, 36]. For a comprehensive overview of WENO and discontinuous Galerkin methods, see [34, 35].

2 Algorithms in Use for Turbulence with Shocks

Starting in the 1990s, many attempts have been made to employ the aforementioned high order shock-capturing schemes (in their original form) for DNS and LES on problems containing discontinuities. Studies [31, 24, 30, 12] indicated that these high resolution, high order shock-capturing schemes are still too dissipative for capturing fine scale turbulence fluctuation. Part of the inaccuracy is due to the fact that DNS and LES computations involve long time integrations. Standard stability and accuracy theories in numerical analysis are not applicable to long time wave propagations and/or long time integrations, especially for finite time steps and finite grid spacings. The original construction of modern shock-capturing schemes were developed for rapidly developing unsteady shock interactions and short time integrations. Any numerical dissipation inherited in the scheme, even for high resolution shock-capturing schemes that maintain their high order accuracy in smooth regions (e.g., fifth or higher order WENO schemes), will be compounded over long time integration leading to smearing of turbulence fluctuations to un-recognizable forms.

In the mid 1990s, Gottlieb & collaborators [14] and Fu & Ma [10] constructed schemes with spectral shock viscosity and group velocity methods, respectively, for limited weak and moderate shock applications. At the same time, hybridizing (switching) between spectral or high order compact schemes and high-resolution shock-capturing methods (switch to shock-capturing methods at discontinuities) was used for shock/turbulence interactions. The switching mechanism can become very complex unless the flows consist of simple shock interactions. For complex shock/turbulence interactions, frequent switching between schemes can create numerical instability. See, e.g., [1]. Recently, a hyperviscosity or artificial fluid approach in conjunction with very high order compact schemes and compact filters has been developed for DNS and LES simulations of turbulence with shocks [8, 11]. Artificial shear viscosity, bulk viscosity, mass diffusivity and thermal conductivity viscosity terms are added to the governing equations. The hyperviscosity approach involves many more tuning parameters than typical high order WENO schemes and is still in the early stage of development. It is not certain that this approach is readily applicable to hypersonic nonequilibrium flow in practical complex geometry settings. Simple test cases with simple shock structure on uniform Cartesian grids have been shown to give accuracy similar to that of high order shock-capturing schemes at the shocks and at the same time give improved resolution at locations of turbulent fluctuation.

Over the last decade, a class of shock-capturing schemes consisting of limiting and filtering with flow sensors [53, 38, 55, 56, 40] has been shown to be more efficient and stable than the switching among two or more schemes approach for shock/turbulence computations. Instead of solely relying on very high order high-resolution shock-capturing methods for accuracy, our filter schemes take advantage of the effectiveness of the nonlinear dissipation contained in good shock-capturing schemes and standard linear filters (and/or high order linear dissipation) as stabilizing mechanisms at locations where needed. The methods consist of two steps, a high order spatial base scheme step and a multistep linear and nonlinear filter. The nonlinear filter consists of the **product** of an artificial compression method indicator or wavelet flow sensor and the nonlinear dissipative portion of a high-resolution shock-capturing scheme (e.g., any TVD, MUSCL, ENO, or WENO scheme). The high order linear filter consists of the product of another flow sensor and a high order linear filter operator. By design, the flow sensors, spatial base schemes and linear and nonlinear dissipation models are stand alone modules. Therefore, a whole class of low dissipative high order schemes can be derived at ease. An advantage of the wavelet flow sensor of the filter method for problems with physical dissipation is that the more scales that are resolved, the less the filter is utilized, thereby gaining accuracy and computation time. In the limit when all scales are resolved, we are left with a "pure" non-dissipative centered high order spatial scheme.

Even with the aforementioned improved control of numerical dissipation, flows containing steady or nearly steady strong shocks on parts of the flow field, and unsteady turbulence with shocklets on other parts of the flow field are difficult to capture accurately and efficiently employing the same numerical scheme, even under the multiblock grid or adaptive grid refinement framework. While sixth-order or higher-order shock-capturing methods are appropriate for unsteady turbulence with shocklets, lower order shock-capturing methods are more effective for strong steady or nearly steady shocks in terms of convergence. In order to minimize the short comings of low order and high order shock-capturing schemes for the subject flows, a multiblock overlapping grid with different orders of accuracy on different blocks has been developed [39] and shown to improve accuracy and efficiency of flows containing mixed steady and unsteady components in complex blunt body geometry settings. Work is underway to apply this ideas to practical test cases.

Even up to the present time, practical application of available schemes for hypersonic nonequilibrium flows is still dominated by second and third-order spatial accuracy with pointwise evaluation of the source terms. The majority of modeling and simulations is confined to steady nonequilibrium aerodynamics on structured grids. A limited number of unsteady hypersonic space vehicle turbulent simulations using second and third-order spatial accuracy have appeared in conference proceedings. See e.g., [37]. Several DNS hypersonic shock boundary-layer studies have been performed with high order methods. See, e.g., [42] and references cited therein. Figure 2.1 summarizes the status of hypersonic flow simulations up to early 2008. Equilibrium flow here refers to problems without source terms.

For ease of complex geometry handling, the current trend in new CFD algorithm development has focused on unstructured grid finite-element and finite-volume methods. Current efforts focus on constructing unstructured grid schemes with shock-capturing capabilities similar to those of their structured counterparts. Most notable are discontinuous Galerkin methods [35]. These high order unstructured grid methods are in the early stages of development for turbulence applications.

It should be noted that one of the major reasons for the limited use of high order finite-volume

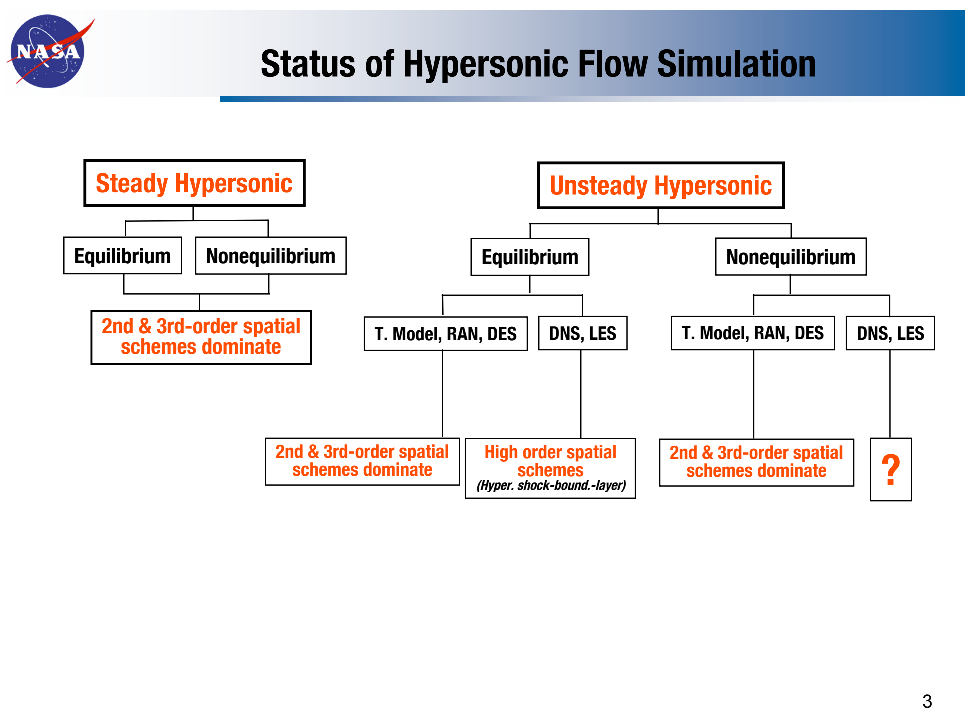

Figure 2.1: Status of hypersonic flow simulations up to early 2008.

schemes for 3-D practical applications is the high computational cost. For example, in 2-D, the finite-volume WENO scheme is 2 to 5 times more expensive than its finite-difference counterpart of the same order, depending on the coding and type of computer. The discrepancy in CPU time cost is even bigger for 3-D. See Shu [34] and references cited therein for a discussion. This reference is also an excellent source on the state-of-the-art of WENO development for finite-volume and finite-difference formulations.

Even within the structured grid framework, hypersonic nonequilibrium flow physics poses many challenges to CFD algorithm development. The next section discusses some of the challenges.

3 Numerical Challenges

3.1 Spurious Numerics Due to Nonlinearity of the Governing Equations and/or Nonlinear Schemes

The sources of nonlinearities that are well known in computational fluid dynamics (CFD) are due to the physics. Examples of nonlinearities due to the physics are convection, diffusion, forcing, turbulence source terms, reacting flows, combustion related terms, or any combination of the above. The less familiar sources of nonlinearities are due to the numerics. There are generally three major sources:

- Nonlinearities due to time discretizations – the discretized counterpart is nonlinear in the time step. Examples of this type are Runge-Kutta methods. If fixed time steps are used, spurious steady-state or spurious asymptotic numerical solutions can occur, depending on the initial condition (IC). Linear multistep methods (LMMs) [4] are linear in the time step, and they do not exhibit spurious steady states. See Yee & Sweby (1991-1997) and references cited therein for the dynamics of numerics of standard time discretizations.

- Nonlinearities due to spatial discretizations – in this case, the discretized counterpart can be nonlinear in the grid spacing and/or the scheme. Examples of nonlinear schemes are the TVD, ENO and WENO schemes. The resulting discretized counterparts are nonlinear (in the dependent variables) even though the governing equation is linear. See [45] and [34] and references cited therein for forms of these schemes.

- Nonlinearities due to complex geometries, boundary interfaces, grid generation, grid refinements and grid adaptations [49]– each of these procedures can introduce nonlinearities even though the governing equation is linear.

Knowledge Gained from Nonlinear Model Problems: In [26, 46, 15, 16, 47, 48, 49, 52, 50, 51, 22, 23, 54], with the aid of elementary examples, Yee and collaborators studied the fundamentals of spurious behavior of commonly used time and spatial discretizations in CFD. These examples consist of nonlinear model ODEs and PDEs with known analytical solutions (the most straightforward way of being sure what is "really" happening with the numerics). They illustrate the danger of employing finite fixed (constant) time steps and finite grid spacings. They were selected to illustrate the following different nonlinear behavior of numerical methods:

- Occurrence of stable and unstable spurious asymptotes **above** the linearized stability limit of the scheme (for constant time steps)

- Occurrence of stable and unstable spurious steady states **below** the linearized stability limit of the scheme (for constant time steps)
- **Stabilization** of unstable steady states by implicit and semi-implicit methods
- Interplay of initial data, grid spacings and time steps on the occurrence of spurious asymptotes
- Interference with the dynamics of the underlying implicit scheme by procedures in solving the nonlinear algebraic equations (resulting from implicit discretizations of the continuum equations)
- Dynamics of the linearized implicit Euler scheme solving the time-dependent equations to obtain steady states vs. Newton's method for solving the steady equation
- Spurious dynamics independently introduced by spatial and time discretizations
- Convergence problems and spurious behavior of high-resolution shock-capturing methods
- Numerically induced & suppressed (spurious) chaos, and numerically induced chaotic transients
- Spurious dynamics generated by grid adaptations

3.2 Numerical Dissipation and Hypersonic Reacting Turbulent Flows

In the modeling of unsteady viscous hypersonic problems containing finite-rate chemistry or combustion, a wide range of space and time scales are often present, over and above the different scales associated with turbulent flows, leading to additional numerical difficulties. One of the main difficulties stems from the fact that most numerical algorithms used in reacting flows were originally designed to solve non-reacting fluid flows. Among many numerical challenges imposed by the subject flows, spatial stiffness due to reacting terms and the presence of turbulence are major stumbling blocks to numerical algorithm development. One of the important numerical issues is that the subject physics cannot tolerate numerical dissipation, but the numerical simulations are unstable without them. Another numerical issue is the proper numerical treatment of a system of highly coupled stiff nonlinear source terms. Based on the first author's experience, three spurious numerics, that are directly tied to the amount of numerical dissipation contained in the chosen scheme and the numerical treatment of source terms can result in

- Possible wrong shock speed and spurious standing waves [26, 46, 15, 16, 22, 23] (due to stiff source terms interacting with numerical dissipation)

  There exist methods that can overcome this difficulty for a single reaction term. One impractical way of minimizing the wrong speed of propagation of discontinuities is to demand orders of magnitude grid size reduction compared with what appears to be a reasonable grid spacing in practice. Another way is to develop efficient, stable, non-dissipative or very low-dissipative adaptive high accurate schemes with non-pointwise evaluation of the reaction terms [22, 23, 16, 9]. In combustion and multifluid mixing applications, front tracking [5] and/or level set method [33] are used to overcome part of the difficulties.

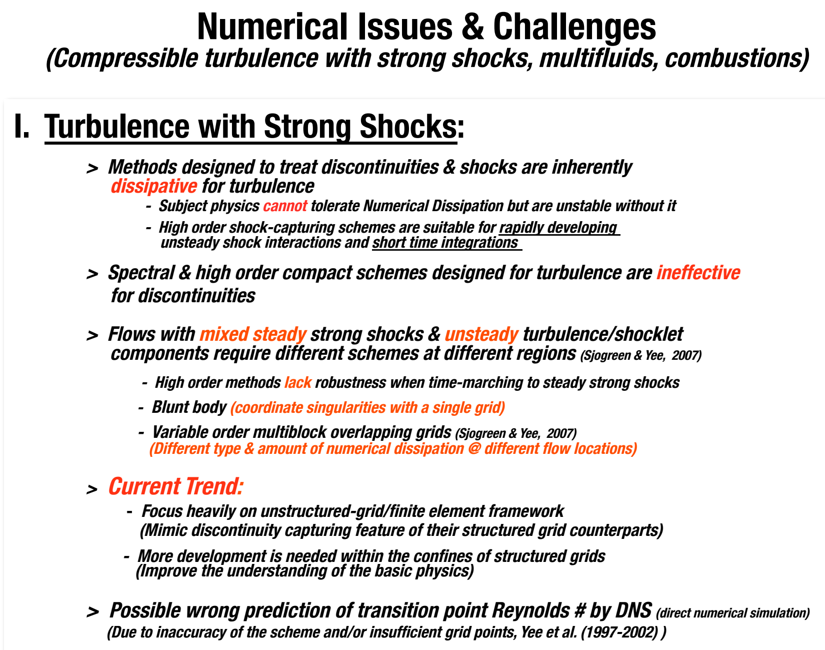

Figure 3.2: Key numerical issues and challenges for turbulence with strong shocks

- Possible spurious steady-state numerical solutions (due to the chosen scheme or the use of a non well-balanced scheme [27])

  A well-balanced scheme (for time-dependent PDEs), as coined by LeVeque [27], refers to schemes that preserve certain non-trivial steady state solutions, if it exists, of the governing equations. For nonequilibrium flows containing non-geometric source terms, we have just begun to address this issue.

- Possible wrong prediction of transition point Reynolds number by DNS (due to inaccuracy of the scheme or insufficient grid points), in addition to smearing of turbulent fluctuations due to numerical dissipation [54].

Figures 3.2 and 3.3 summarize some of the key numerical challenges for hypersonic turbulent flow simulations.

3.3 Multi-Fluid Flows

For material mixing, almost all high order shock-capturing methods exhibit oscillations at material interfaces. Figure 3.4 shows the behavior of a second-order TVD scheme, several WENO schemes compared with the aforementioned filter approach for a 1-D two-fluid mixing shock tube test case containing discontinuities using the same grid. It indicates that the higher the order of the shock-capturing scheme, the more pronounced the oscillation at the material interface. With the filter approach using the same shock-capturing dissipation, the oscillations at interfaces are less pronounced.

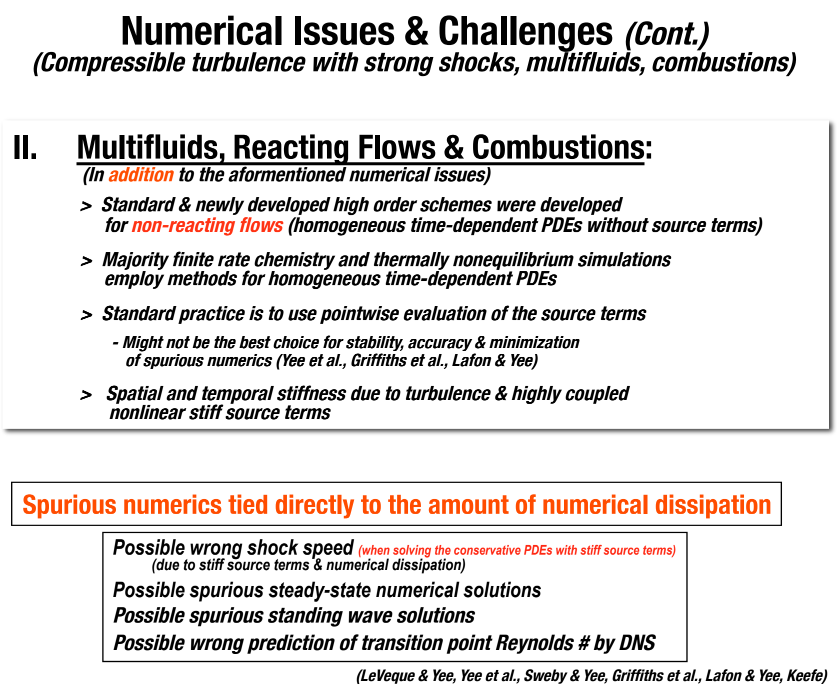

Figure 3.3: Key numerical issues and challenges for reacting flows.

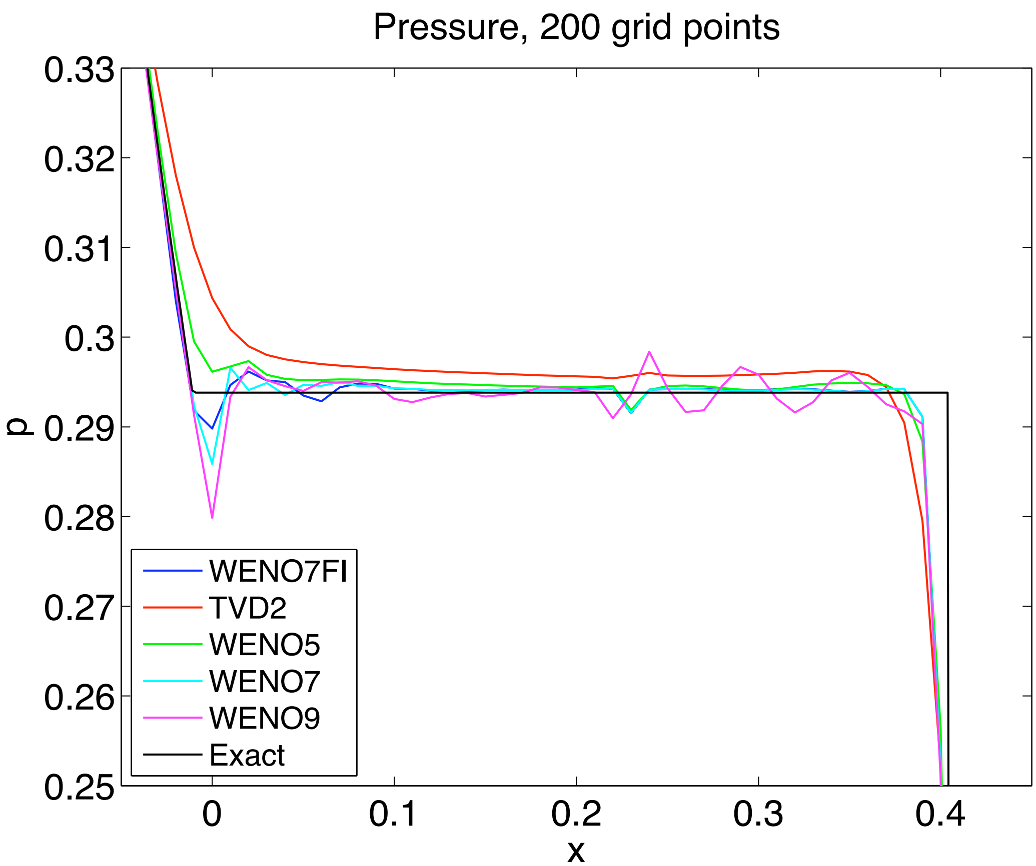

Figure 3.4: 1-D two fluid mixing problem containing discontinuities: Comparison of a second-order TVD (TVD2), WENO5, WENO7, WENO9 (5th, 7th and 9th-order WENO) and a filter scheme using a dissipative portion of WENO7 (WENO7fi)

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