Quantification of Numerical Uncertainty in DNS Simulations of Compressible Turbulence with Strong Shocks – *A Dynamics of Numerics Approach*

White Paper for DOE/ASCR Workshop on Turbulent-Flow Simulations at the Exascale

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1 Challenges

The proposed DOE exascale computing is projected to facilitate computational simulation of physical phenomena at new levels of accuracy, fidelity, and scale, as well as allowing innovative capabilities for in-depth computational intensive analysis such as uncertainty quantification. These computational stringent requirements are particularly important for predictive science of complex (magnetized) compressible turbulent flows containing strong shock waves and stiff source terms. It is the interplay of turbulence in variable density media with magnetic fields and with shocks that makes the prediction and control of system behavior so difficult in many engineering and science applications. Turbulence and shocks are able to amplify the magnetic field through dynamo action and compression. The field amplification would in turn change the scaling and critical conditions for turbulence development as well as the shock jump conditions.

Numerical simulation is challenging due to the conflicting requirements for numerical methods to be accurate enough to resolve the small scales of turbulence but robust enough to handle shock waves without generating spurious numerical noise. In compressible turbulent flows containing stiff source terms, the constructions of numerical schemes for (a) stable and accurate simulation of turbulence with strong shocks, and (b) obtaining correct propagation speed of discontinuities for stiff reacting terms share one important ingredient - minimization of numerical dissipation while maintaining numerical stability. This dual requirement to achieve both numerical stability and accuracy is most often conflicting for existing schemes that were designed for flows without stiff source terms. For stiff reactions it is well known that the wrong propagation speed of discontinuities occurs, see LeVeque & Yee [2] and Yee et al [7]. Schemes to ensure the correct propagation speed of discontinuities for systems of stiff reacting flows remain a challenge for algorithm development.

2 Relevance, Approach and Objective

Yee et al. and collaborators worked extensively on nonlinear behavior of standard spatial and temporal discretizations related to the predictability and reliability of data-limited complex multiscale nonlinear simulations via the dynamical system approach. (See [6] and references cited therein). Examples reported in [2, 4, 1, 6] indicated that spurious numerical solutions in the form of "spurious steady states, spurious periodic solutions, spurious limit cycles, spurious chaos, and spurious chaotic transient/turbulence" can be independently introduced by temporal and spatial discretizations. These dynamics of numerics are especially important to data-limited multiscale turbulent flows and laminar transition to turbulence/chaotic flows by direct numerical simulations (DNS). Due to inaccuracy of the scheme, insufficient grid point resolution and sensitivity to initial data on turbulent flows, their studies showed [6] that it is possible to incorrectly predict the transition point Reynolds number by DNS. "Spurious Numerics" here means numerical solutions that are solutions of the nonlinear discretized equations, but they are not solutions of the chosen governing equation model. This approach is very different from the standard uncertainty quantification and error bound estimate control which is based on local linearized analysis as the time step and grid spacing approach zero.

Numerical Chaos, Chaotic Transient & Flow Transition by Direct Simulation

Aside from the inherent chaotic and chaotic transient behavior in some physical systems, numerics can independently introduce and suppress chaos as well as chaotic transients. Loosely speaking, a chaotic transient behaves like a chaotic solution. A chaotic transient can occur in a continuum or a discrete dynamical system. One of the major characteristics of a numerically induced chaotic transient (numerical chaos) is that if one does not integrate the discretized equations long enough, the numerical solution has all the characteristics of a chaotic solution. The required number of integration steps might be far beyond those found in standard computational physics practice before the numerical solution can get out of the chaotic transient mode. A possible numerically induced chaotic transient is especially worrisome in DNS of the transition from laminar to turbulent flow. With currently available computer power, the numerical simulation can result in chaotic transients indistinguishable from sustained turbulence, yielding a spurious picture of the flow for a given Reynolds number. Consequently, it casts some doubt on the reliability of numerically predicted transition points and chaotic flows. It also influences the true connection between chaos and turbulence.

Employing theory from nonlinear dynamics, Yee and collaborators [2, 4, 1, 6] concentrate only on how well numerical schemes can mimic the solution behavior of the underlying PDEs. The possible discrepancy between the chosen model and the real physics and/or experimental data is set aside. Assuming a known physical bifurcation or transition point and using the same initial condition (IC) and boundary condition (BC), Fig. 1 illustrates the schematic of four possible spurious bifurcations due to constant time steps and constant grid spacings for nonlinear numerical simulations. This work of Yee and collaborators illustrates all of the possible scenarios of spurious bifurcations indicated on the schematic diagram. The observed spurious behavior related to under-resolved grid cases is particularly relevant to DNS and large eddy simulation (LES). Spatial resolutions in DNS and LES are largely dictated by the computer power.

Objective: With the advent of exascale computing, theory of nonlinear dynamics will be able to be utilized more fully to complement the traditional linearized stability theory to improve predictability and reduce numerical uncertainty for compressible turbulence flows containing strong shock waves and stiff source terms. Due to sensitivity to initial data by both turbulence and chaotic flows, shadowing Lemma for both the continuum and the discretized counterparts [3] needed to be utilized. The objective of this work is to utilize recent advances in theory of dynamical systems, especially Lyapunov Exponents and Shadowing Lemma approaches to minimize numerical uncertainty in DNS of the subject compressible turbulent flows. These new procedures in the quantification of uncertainty of turbulence simulations are orders of magnitude more computational intensive than standard turbulent flow computations.

3 Impact

Ensuring a higher level of confidence in the predictability and reliability of these numerical simulations could play a major role in furthering the design, understanding, and affordability of topics that are of direct relevance to the DOE basic energy science and technology research, including Energy Efficiency, Extreme Environments (e.g., computational modeling of supernova type II explosions and supersonic turbulence in star-forming molecular clouds), Combustion (e.g., multi-scale simulation of scramjets and internal combustion engines), and Transportation (virtual design of drag on fuel transport in pipes, ducts, and vehicles). We believe the nonlinear dynamical approach can compliment the existing uncertainty quantification in numerical simulations. It should also be an integral part of code development and code Verification & Validation as well as code Certification efforts.

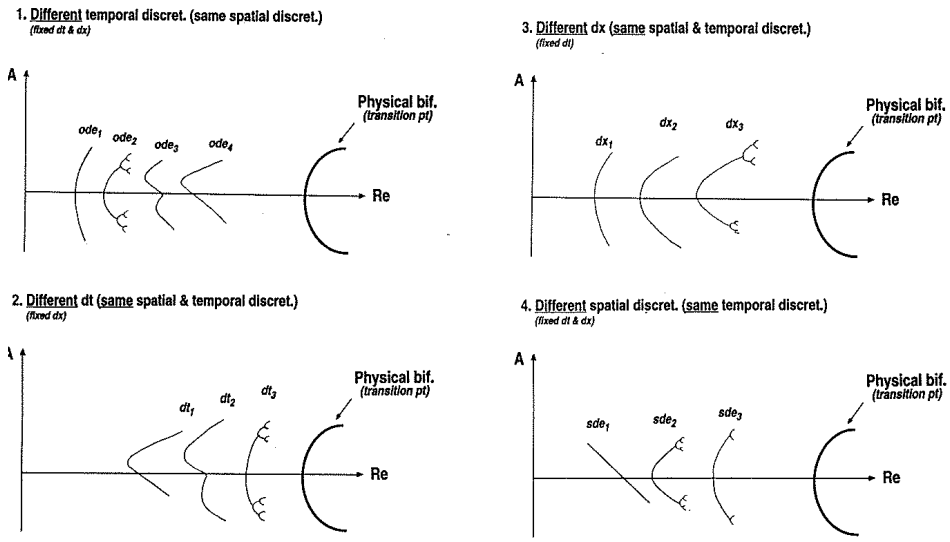

Figure 1: Schematic of possible spurious bifurcation (assume a certain physical transition with same IC & BC) for constant time steps and grid spacings as a function of Reynolds number Re and some norm solution A. (1) Different temporal discretizations ode_1, ode_2, ode_3 and ode_4 (same spatial discretization and the same constant dt and dx). (2) Different constant time steps dt_1, dt_2, dt_3 and dt_4 (same temporal and spatial discretizations, and the same constant dx). (3) Different constant grid spacings dx_1, dx_2 and dx_3 (same spatial and temporal discretizations, and the same constant dt). (4) Different spatial discretizations sde_1, sde_2 and sde_3 (same temporal discretization and the same constant dt and dx).

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