8th. World Congress on Computational Mechanics (WCCM8)
5th. European Congress on Computational Methods in Applied Sciences and Engineering (ECCOMAS 2008)
June 30 – July 5, 2008
Venice, Italy

ON VERIFICATION & VALIDATION OF TURBULENT FLOW SIMULATION MODELS

Fernando F. Grinstein[1]

[1] *Applied Physics Division, Los Alamos National Laboratory*
MS-B259, Los Alamos, NM 87545
fgrinstein@lanl.gov

Key Words: Multiple-Scale Physics And Computation, Minisymposia on Accomplishments and Challenges in Verification & Validation

ABSTRACT

Turbulent flows are of considerable importance in many applications in engineering, geophysics, meteorology, and astrophysics, where experiments based on predictive numerical simulations play a fundamental research role. A crucial validation aspect of turbulent flow simulations, is that of adequately characterizing the conditions in both, numerical and reference experiments. Often, the assumption made in applied turbulence research is that initial condition effects eventually wash-out (loss of memory) as the turbulence develops. However, a growing body of fundamental research (e.g. [1]) indicates that only very special turbulent flows are truly self-similar. In this context, it is thus crucially important to recognize the inherently intrusive nature of both, computed and laboratory observations based on turbulent phenomena.

Relevant flow characterization issues relate to the treatment of the unresolved features at the subgrid scale (SGS) level – within a computational cell – and at the supergrid scale (SPGS) level – beyond computational boundaries (e.g., [2]); such SGS and SPGS information must be prescribed for closure of the equations solved numerically. SGS models appear (explicitly or implicitly) as additional source terms in the *modified* flow equations (solved by the numerical solutions being calculated), while SPGS models provide the necessary set of boundary conditions that must be prescribed to ensure unique well-posed solutions. From this perspective, the observational (simulation) process is inherently affected (determined) by the (unresolved SGS and SPGS) information prescription process. On the other hand, observables in laboratory experiments are always characterized by the finite space/time scales of the instrumental resolution of measuring/visualizing devices. Ultimately, there is also a finite extent to which laboratory observations can be made in a non-intrusive fashion due to basic uncertainty principles. Laboratory experiments are constrained as well by finite dimensions of the facilities and actual flow boundary conditions are typically insufficiently characterized. The possible transient and/or long-term effects of the particular initial conditions of (computational or laboratory) experiments need also be addressed.

Capturing the dynamics of all relevant scales of motion, based on the numerical solution of the Navier–Stokes equations, constitutes direct numerical simulation (DNS), which is prohibitively expensive in the foreseeable future for most practical flows of interest at moderate-to-high Reynolds number. The Reynolds-averaged Navier–Stokes (RANS)

approach, with averaging typically carried out over time or across an ensemble of equivalent flows, is typically employed for turbulent flows of industrial complexity. Large eddy simulation (LES) has become the effective intermediate approach between DNS and RANS, capable of simulating flow features that cannot be handled with RANS, such as significant flow unsteadiness and strong vortex-acoustic couplings, and providing higher accuracy than RANS at reasonable cost (e.g., [3]). LES is based on the expectation that the physically meaningful scales of turbulence can be split into two groups: one consisting of the resolved geometry and regime specific scales (so-called energy containing scales), and the other associated with the unresolved smallest eddies, for which the presumably more-universal flow dynamics is represented with subgrid scale (SGS) closure models. Adding to the physics based difficulties in developing and validating SGS models, are truncation terms due to discretization that are comparable with SGS models in typical LES strategies [4]. Implicit LES (ILES) [5] effectively addresses the seemingly insurmountable issues posed to LES by under-resolution by relying on SGS modeling and filtering provided implicitly by physics capturing numerics of certain high resolution finite-volume numerical algorithms (e.g., flux-corrected transport, the piecewise parabolic method, and total variation diminishing algorithms). ILES analysis focuses on the modified flow equations satisfied by the numerically calculated solutions, which provide a framework to reverse engineer physically desirable features into the numerics design.

An overview of LES verification and validation issues involved will be presented, and relevant SGS, SPGS, and discretization aspects will be addressed in this context. Ongoing verifications studies focusing on SGS issues relevant to the simulation of transition to turbulence in the Taylor-Green vortex case will be presented. Difficult SPGS aspects of turbulent flow initial/boundary condition characterization and modeling in validation studies will be illustrated in selected flow problems of practical interest, including complex flow simulation in multi-swirler combustors and urban scenarios.

REFERENCES

[1] George, WK, “Recent advancements toward the understanding of turbulent boundary layers,” *AIAA Journal*, ; v.44, no.11, p.2435-2449, 2006.
[2] Grinstein, F.F, 2004, Ed., “Boundary Conditions for LES”, *AIAA Journal*, **42**, 437-492.
[3] Sagaut P.,Large Eddy Simulation for Incompressible Flows, 3rd Edition, Springer, New York, 2005
[4] Ghosal, S., 1996, “An analysis of numerical errors in large-eddy simulations of turbulence”. *J. Comput. Phys*. **125**, 187-206.
[5] Grinstein, F.F., Margolin, L.G. and Rider, W.J., Eds., *Implicit Large Eddy Simulation: Computing Turbulent Flow Dynamics*, Cambridge UP, 2007.