On integrating large eddy simulation and laboratory turbulent flow experiments

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Critical issues involved in large eddy simulation (LES) experiments relate to the treatment of unresolved subgrid scale flow features and required initial and boundary condition supergrid scale modelling. The inherently intrusive nature of both LES and laboratory experiments is noted in this context. Flow characterization issues becomes very challenging ones in validation and computational laboratory studies, where potential sources of discrepancies between predictions and measurements need to be clearly evaluated and controlled. A special focus of the discussion is devoted to turbulent initial condition issues.

Keywords: turbulent flow experiments; large eddy simulation; subgrid scales; initial conditions; boundary conditions

1. Background

Turbulent flows are of considerable importance in many areas of engineering, geophysics, meteorology and astrophysics. Availability of effective predictive tools is a crucial aspect in the applications. Laboratory studies typically demonstrate the end outcome of complex nonlinear three-dimensional physical processes with many unexplained details and mechanisms. Flow experiments based on numerical simulations carried out with precise control of initial conditions (ICs) and boundary conditions (BCs) are ideally suited to provide insights into the underlying dynamics of laboratory observations. A crucial aspect in this collaborative context is that of adequately characterizing the laboratory and numerical experiments, so that potential sources of discrepancies can be clearly evaluated and controlled.

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 practical flows of interest at moderate to high Reynolds numbers ($Re$). On the other end of computer simulation possibilities, the Reynolds-averaged Navier–Stokes (RANS) approach, with averaging typically carried out over time, homogeneous directions or across an ensemble of equivalent flows, is typically employed for turbulent flows of industrial complexity. Large eddy simulation

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(LES; Sagaut 2006; Grinstein et al. 2007) 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. LES is based on the expectation that physically meaningful scales of turbulence can be split into two groups: one consisting of the resolved geometry and regime-specific scales—the 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.

Relevant issues relate to the modelling of the unresolved flow conditions at the SGS level, within a computational cell, and at the supergrid scale (SPGS), at initialization and beyond computational boundaries. 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 BCs that must be prescribed to ensure unique well-posed solutions. From this perspective, it is clear that the simulation process is inherently determined by the SGS and SPGS information prescription process. On the other hand, observables in laboratory experiments are always characterized as well by finite dimensions of the facilities and actual flow conditions at its boundaries. It is thus important to recognize the inherently intrusive nature of both numerical and laboratory experiments.

The possible transient and/or long-term effects of the particular ICs of computational and laboratory experiments need also be addressed. In what follows, an overview of SGS and SPGS issues is presented, and relevant discretization aspects are noted. The discussion then focuses on fundamental turbulent IC characterization and modelling difficulties arising when attempting to integrate LES and laboratory experiments in complex flow problems of current practical interest.

2. Subgrid scale issues

In LES we are constrained to simulate a flow with the smallest characteristic resolved scale determined by a resolution cut-off wavelength determined by a spatial-filtering process. Effective analysis of LES methods can be based on a formal procedure called modified equation analysis (MEA)—see Grinstein et al. (2007) and references therein. To simplify the MEA discussion, we focus here on the conceptually simplest material mixing case, that of incompressible flow with scalar mixing. The modified LES equations (satisfied by the numerically calculated solutions) are the following:

\[
\partial_t \langle \bar{v} \rangle + \nabla \cdot (\bar{v} \otimes \bar{v}) + \nabla \bar{p} - \nu \nabla \cdot \bar{S} = -\nabla \cdot \sigma_v + t_v
\]

and

\[
\partial_t \langle \bar{\theta} \rangle + \nabla \cdot (\bar{\theta} \otimes \bar{v}) - \kappa \nabla^2 \bar{\theta} = -\nabla \cdot \sigma_\theta + t_\theta,
\]

where the bar denotes a formal spatial filtering procedure; \( v \) is the solenoidal velocity field; \( \theta \) is a conserved material scalar concentration; \( \nu \) and \( \kappa \) denote momentum and material diffusivity, respectively; and \( t_v \) and \( t_\theta \) address effects of
discretization and commutation between differentiation and filtering. To ensure closure of the equations in the filtered unknowns, explicit models for 
\[ \sigma_v = \bar{v} \otimes \bar{v} - \bar{v} \otimes \bar{v} \] and 
\[ \sigma_\theta = \theta \bar{v} - \bar{v} \otimes \bar{v} \] have to be provided.

In the absence of an accepted universal theory of turbulence to solve the problem of SGS modelling, the development and improvement of such models must include the rational use of empirical information and pragmatic practice. Several strategies to the problem of SGS modelling have been attempted (Sagaut 2006). After nearly four decades of intense research on the LES of turbulent flows based on eddy-viscosity models, there is now consensus that such an approach is subject to fundamental limitations. Eddy-viscosity models are able to reproduce the SGS dissipation quite well, but not the SGS forces entering the momentum equation, thereby making this approach less suited for complex high Re flows that are usually poorly resolved. The most recent efforts have focused on developing mixed models, combining in essence the dissipative eddy-viscosity models with the more accurate but less stable scale-similarity models, providing a more accurate SGS force approximation. The results from such mixed models have been mostly satisfactory, but their implementation and computational complexity have limited their popularity.

A crucial practical computational aspect is the need to distinctly separate the effects of filtering and SGS reconstruction models from the unavoidable implicit ones due to discretization. Indeed, it has been noted that, in typical LES strategies, \( t_v \) and \( t_\theta \), which are truncation terms due to discretization and filtering, have contributions directly comparable with those of the explicit models (Ghosal 1996). Seeking to address the seemingly insurmountable issues posed to LES by under-resolution, some researchers have explored the possibility of using the SGS modelling and filtering provided implicitly by the numerics; this is generally denoted as numerical LES by Pope (2004). Arbitrary numerics will not work in this endeavour: good or bad SGS physics can be built into the simulation model depending on the choice and particular implementation of the numerics. MEA provides the natural framework to reverse-engineer desirable features into the numeric design.

Implicit LES (ILES) was first proposed by Boris (1990) as the monotone integrated LES approach (MILES). ILES incorporates the effects of the SGS physics on the resolved scales through functional reconstruction of the convective fluxes with certain high-resolution non-oscillatory finite volume (NFV) algorithms; this includes popular physics capturing methods, such as flux-corrected transport, the piecewise parabolic method and total variation diminishing algorithms (Grinstein et al. 2007).

In the context of forced isotropic turbulence simulations, comparisons of instantaneous probability density functions of SGS viscosities associated with typical LES and ILES (Fureby & Grinstein 1999) show similar behaviours sensitive to the actual explicit or implicit SGS models involved. Taylor–Green vortex studies (Drikakis et al. 2007) demonstrate the robust capabilities of ILES in simulating transition to turbulence and turbulence decay (e.g. figure 1), and indicate that SGS models associated with LES and ILES act very similarly in predicting Re-independent regimes asymptotically attained with increasing grid resolution. Extensive ILES verification and validation studies of turbulent flows in engineering, geophysics and astrophysics have been reported (Grinstein et al. 2007). For regimes driven by large-scale flow features, for
which LES is designed, implicit models associated with NFV methods have been shown to be capable by themselves ($\sigma \equiv 0$) to emulate SGS physics effects on statistics of turbulent velocity fluctuations. Major features of the flow physics can be captured with locally adaptive dynamic NFV methods: (i) the small-scale
anisotropy of high-Re turbulent flows (for e.g. line vortices and shocks), (ii) the viscosity-independent dissipation characteristic of the turbulent cascade, and (iii) the inherently discrete dynamics of finite-scale laboratory observables. By focusing on inertially dominated flow dynamics and regularization of the under-resolved flow, ILES follows on the precedent of using NFV methods for shock capturing—requiring weak solutions and satisfaction of an entropy condition.

Depending on grid resolution and flow regimes involved, additional explicit SGS modelling \((\sigma \neq 0)\) may be needed with ILES to address SGS-driven flow physics, e.g. near walls, and when simulating backscatter, mixing and chemical reaction. A major research focus is on evaluating the extent to which the particular SGS physical effects can be implicitly modelled as the turbulent velocity fluctuations, recognizing when additional explicit models and/or numerical treatments are needed, and when so, addressing how to ensure that mixed explicit and implicit SGS models effectively act in a collaborative rather than interfering fashion.

3. Supergrid scale issues

Although SGS issues have motivated intense research, less attention has been devoted to the equally relevant SPGS BC modelling aspects, the importance of which is often overlooked. Because SPGS choices select flow solutions, emulating particular flow realizations demands precise characterization of initial and asymptotic conditions, as well as conditions at solid and other relevant boundaries. The flow characterization issue is a particularly challenging one when laboratory realizations are involved because the available SPGS info is typically incomplete. The impact of SPGS specifics in driving the flow dynamics has been recognized in laboratory experiments (e.g. Hussain & Zedan 1978; Gutmark & Ho 1983; George 1990; Li & Gutmark 2006), and clearly noted: ‘unlike the theoretician, the experimentalist already knows the solution, for it is the flow he has realized. His objective is to find which equations and which boundary and ICs his solution corresponds to, and then to compare them and his results with those dealt with by the theoretician’ (George 1990).

In studying flows developing in space and time, the simulated solution must be initialized, and only a finite spatial portion of the flow can be investigated. We must ensure that the presence of artificial open boundaries adequately bounds the computational domain without polluting the solution in a significant way, (e.g. Poinset & Lele 1992; Colonius et al. 1993; Grinstein 1994). Physical issues involved in the BC analysis involve issues of numerical consistency and difficulties in mathematically prescribing actual physical models. To ensure that specifically desired flow realizations are simulated, the BC models must be capable of: (i) prescribing effective turbulent ICs, (ii) emulating eventual feedback effects from presumed virtual flow events outside of the finite-sized computational domains at open inflow, outflow and cross-stream boundaries (Grinstein 1994), (iii) enforcing appropriate flow dynamics and energy transfer near walls (Spalart et al. 1997; Kong et al. 2000; Fureby et al. 2004; Sagaut et al. 2004; Sidwell et al. 2006), and (iv) minimizing spurious numerical reflections at all computational boundaries through use of suitable discretized representations.
Owing to discretization, derivatives can only be approximated at the boundaries. Additional numerical BCs (NBCs) need to be specified to ensure closure of the discretized system of equations. NBCs are distinct from the discretized representations of the physical BCs (PBCs) required to uniquely define a solution of the continuum fluid-dynamical problem traditionally used as reference. The goal is to ensure that the expected behaviour of the latter solution outside the computational domain be properly and consistently imposed on the solution inside. The consistency requirement demands that, in the continuum limit, the NBCs be compatible with the flow equations and PBCs, in such a way that they do not generate new BCs that over-specify the fluid dynamical problem. For hyperbolic equations, a relatively simple framework for BC implementation focuses on the terms of the flow equations containing derivatives with respect to the (local) direction perpendicular to the boundary (Thompson 1990). Despite its limitations, being one-dimensional and based on characteristic analysis (Colonius et al. 1993), this strategy offers a systematic approach (Poinsot & Lele 1992) to the problem of imposing PBCs and NBCs in practical simulations.

4. Inflow and ICs

Traditionally, the loss of memory assumption has been made in turbulence research, i.e. IC effects eventually wash-out as the turbulence develops. However, a growing body of fundamental research indicates that only very special turbulent flows are truly self-similar. The sensitivity to ICs has been extensively reported in recent years (e.g. Slessor et al. 1998; George & Davidson 2004; Ramaprabhu et al. 2005). Robustness of simulation results is an important unsettled issue in this context: if the IC information contained in the filtered-out smaller and SGS spatial scales can significantly alter the evolution of the larger scales of motion and practical integral measures, then the use of any LES for their prediction as currently posed is dubious and not rationally or scientifically justifiable. The selected case studies that follow illustrate crucial IC characterization and modelling difficulties encountered when integrating LES and laboratory experiments in complex flow problems of interest.

(a) Characterizing inflow

To illustrate typical PBC prescription requirements, we focus on the open BC problem; see Poinsot & Lele (1992) for a discussion of typical requirements for other cases. The number of inflow/outflow open BCs required to ensure well-posedness and to completely determine the flow solution within a given finite domain is well known for both Euler and Navier–Stokes equations from theoretical analysis (e.g. Strikwerda 1977; Oliker & Sundstrom 1978), and are listed for reference in table 1.

For the sake of discussion, consider the three-dimensional Euler equations, and the problem of specifying the necessary open BCs in the \(x\)-direction, which we assume to be the streamwise direction. At the inflow boundary, the four inflow PBCs can be chosen to specify the free-stream velocity components, plus one additional prescribed quantity, e.g. mass density, temperature or pressure. The additional viscous inflow BCs needed for the case of the Navier–Stokes equations are expected to have small effects on inflow characterization (Poinsot & Lele 1992).
Different inflow PBC choices providing closure are not equivalent, i.e. they do not necessarily lead to the same solution. This is a very important aspect to keep in mind when comparing computational or laboratory experiments with presumably very similar, but not necessarily identical, BCs. Non-reactive General Electric Aircraft Engines (GEAE) LM-6000 swirl combustor simulations (Kim et al. 1999; Grinstein & Fureby 2004) are used in the following to exemplify this issue. At the subsonic combustor inlet, four primary flow variables can be prescribed through Dirichlet conditions, and at least one other physical quantity must be allowed to float. The available information from the GEAE LM-6000 laboratory studies consisted of the mean (time-averaged) profiles of the velocity components at a selected transverse inlet plane, where turbulent velocity fluctuations were reportedly low. Standard temperature and pressure conditions were expected, but there were no indications from the laboratory data on whether choosing any particular fourth flow variable to specify at the inflow—other than the velocity components—was to be preferred.

Inflow turbulence was either emulated with broad-band random fluctuations (Kim et al. 1999) or neglected altogether (Grinstein & Fureby 2004) in the LM-6000 simulations. Kim et al. (1999) chose to prescribe inlet velocity components and temperature (S. Menon ca 2001, personal communication). Two other inlet BC approaches were tested by Grinstein & Fureby (2004) based on: (i) prescribing the inflow velocity components and mass density, and allowing pressure and temperature to float through a characteristic-analysis-based condition (Poinsot & Lele 1992), and (ii) allowing the inlet radial velocity to float (suggested by Z. Rusak ca 2001, personal communication). Comparison of mean centreline velocity results in figure 2a, from non-reactive LES by Kim et al. (1999) and by Grinstein & Fureby (2004) clearly demonstrate that the near-inlet combustor flow can be quite sensitive to the choice of inlet floating condition; on the other hand, figure 2b indicates that LES predictions become fairly robust once adequately similar inflow BCs are involved.

(b) Turbulent inflow

As noted, the sensitivity of turbulent flows to particular IC choices is now well recognized (George & Davidson 2004). Far-field portions of turbulent flows remember their particular near-field features, and the mechanism by which the transition from ICs to particular associated asymptotic flow occurs involves unsteady large-scale coherent-structure dynamics, which can be captured by LES but not by single-point closure turbulence modelling (e.g. RANS). As a very particular consequence, starting with the typical availability of single-point statistical data, there is no unique way to reconstruct a three-dimensional unsteady velocity field with turbulent eddies to define realistic inflow BCs; such data is typically insufficient to parametrize turbulent inflow BCs for the LES of inhomogeneous flows, e.g. Druault et al. (2004).
Approaches to modelling turbulent inflow are extensively surveyed in Sagaut (2006). Because the flow is more or less driven by inflow conditions, prescribed realistic turbulent fluctuations must be able to achieve some sort of equilibrium with imposed mean flow and other BCs. The inherent inability to carry out this inflow BC reconstruction properly in the simulations has led to using a transition inflow region where imposed flow conditions evolve into realistic turbulent velocity fluctuations after allowing for feedback effects to occur as the simulation progresses. The challenge is how to minimize the length of this developmental region, since its presence adds to overall computational cost through additionally required grid points and data processing involved. At a more fundamental level, however, using an artificial transitional inflow region may not be adequate to emulate the actual turbulent inflow conditions involved—a serious issue if ICs are not forgotten. Typical difficulties with characterizing and modelling turbulent inflow conditions in recent practical simulations are exemplified in what follows (figure 2).

The upwind atmospheric boundary layer characterization directly affects the inflow condition prescription required in urban scenario simulations. Wind fluctuation specifics are major factors in determining urban contaminant transport. The important length-scales (tens of metres to kilometres) and time scales (seconds to minutes) in wind gusts can in principle be resolved. However, the flow data from actual field trials or wind-tunnel experiments are typically inadequate and/or insufficient to fully characterize the boundary layer conditions required in the urban flow simulation model. In the recent simulations of flow and dispersal over an urban model (cube arrangement) in wind tunnels (Patnaik et al. 2007), the available datasets from the laboratory experiments consisted of high

Figure 2. LES and MILES of a swirl combustor flow. Sensitivity of the simulated centreline axial velocity within a combustor to actual choices of steady inflow BCs; streamwise variable is scaled with inlet diameter $R$. Results from Grinstein & Fureby (2004) were obtained with two different codes based on MILES and the One-Equation-Eddy-Viscosity-Model (OEEVM) LES, respectively, and compared with previous (dynamic Smagorinsky) LES results from Kim et al. (1999). (a) Centreline axial velocity $u/U_0$; Kim et al. (1999); solid line, fine grid; circles, coarse grid (fixed $T$ and $u_{rad}$); Grinstein & Fureby (2004); black curve, MILES (fixed $p$ and $u_{rad}$); green curve, MILES (fixed $P_o$ and floating $u_{rad}$); red curve, OEEVM (fixed $p$ and $u_{rad}$). (b) Centreline axial velocity (fixed $T$ and $u_{rad}$ at inlet); Kim et al. (1999); solid line, fine; circles, coarse; Grinstein & Fureby (2004); black solid and stripped lines, MILES; red solid and stripped lines, OEEVM.

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quality, spatially dense (but not time-resolved) single-point statistical data. The inflow velocity in the simulations modelled mean profiles and superimposed fluctuations. An iterative process was used, in which a phenomenological unsteady-wind model was calibrated to provide a fit to the experimentally observed r.m.s. values at locations upstream of the urban model. Agreement was achieved by adjusting amplitude, spatial wavelength and temporal frequency of the imposed wind fluctuations in an unsteady-wind model. This approach provided a practical approximation to the turbulent inflow BC specification problem consistent with the available laboratory data. Particularly relevant insights follow from this work, when comparing predicted and measured volume fractions of a tracer scalar in the first few urban model canyons using various different inflow condition models, as shown in figure 3. Prescribing some reasonable inflow turbulence, as opposed to prescribing steady inflow, was found to be critical. On the other hand, the fluid dynamics within the cube arrangement, i.e. beyond the first canyon, becomes somewhat insulated from flow events in the boundaries, i.e. it is less dependent on the precise details of the modelled inflow turbulence and largely driven by the urban geometry specifics within the urban arrangement.

As noted above, using an artificial transitional inflow region to emulate turbulent inflow physics may not be an option. This is the case in the context of simulation of complex combustor flows with multi-swirl inlets (Grinstein et al. 2002; Grinstein & Fureby 2004; Li & Gutmark 2006; Fureby et al. 2007), where inlet length controls the coupling between swirl motion and sudden expansion, and thus cannot be arbitrarily varied to accommodate an inflow BC implementation. Promising pseudo-deterministic approaches propose generating an interface of inflow BCs for LES based on the use of two-point statistics and combined linear stochastic estimation and proper orthogonal decomposition techniques (Druault et al. 2004). A linear stochastic estimation approach was used to post-process the multi-swirl inlet velocity data (Verfaillie et al. 2006). It enabled the reconstruction of the complete coherent flow fields at the

Figure 3. (a) MILES studies of flow and dispersion over an urban (cube arrangement) model, from Patnaik et al. (2007). (b) Colours correspond to predicted and measured dispersal of tracer volume fractions in first few urban canyons indicated by (a). Wind-tunnel experiments, symbols simulations; solid curve, modelled inflow turbulence; dashed curves, steady inflow (no turbulence).
multi-swirler outlet from the knowledge of only few near-field acoustic signals, thus providing a promising effective tool for laboratory data reduction to formulate turbulent inflow BCs for practical LES combustor studies. However, hybrid approaches attempting to represent interface physics with effective BCs should somehow also include the effects of flow couplings across the BC plane on the development of acoustic or combustion instabilities. Depending on the importance of the latter couplings, and on the specific questions that the simulations are meant to address, carrying out the more-expensive larger-system LES, including the simulation of the complex inlet geometry flow, may be unavoidable (Fureby et al. 2007).

(c) Intertwined SGS and SPGS issues

In many applications of interest, SGS and SPGS issues cannot be dealt with independently. This is typically the case when studying near-wall flows or material mixing driven by under-resolved multi-scale turbulent velocity fields, where multi-scale resolution issues become compounded with the inherent sensitivity of turbulent flows to ICs. An example is turbulent mixing generated by shock waves via Richtmyer–Meshkov instabilities (RMIs), where vorticity is introduced at material interfaces by the impulsive loading of a shock wave (e.g. Hill et al. 2006; Youngs 2007). A critical feature of this impulsive driving is that the turbulence decays as dissipation removes kinetic energy from the system. RMIs add the complexity of shock waves and other compressible flow effects to the basic physics associated with mixing; compressibility further affects the basic nature of material mixing when mass density and material mixing fluctuation effects are not negligible. Because RMIs are shock-driven, resolution requirements make DNS unpractical, even on the largest supercomputers. State-of-the-art simulations use hybrid methods that switch between shock capturing schemes and conventional LES, depending on local flow conditions (e.g. Hill et al. 2006) or ILES (e.g. Cohen et al. 2002; Youngs 2007).

The unique combination of shock and turbulence emulation capabilities supports direct use of ILES as effective computer simulation anzatz in RMI research. The particular ILES strategy exemplified here is based on a nominally inviscid simulation model, which solves the conservation equations for mass density ($\rho$), momenta ($\rho u_i$), total energy and partial material densities convected as separate scalars. We use the radiation adaptive grid Eulerian (RAGE) code (Gittings et al. 2006), which solves the multi-material compressible Euler equations using a second-order Godunov scheme, with various available numerical options for gradient terms (limiters) and material interface treatments; min-mod (MM) and Van Leer (VL) limiters can be used in conjunction with an interface preserver (IP) to limit the numerical spread of material concentrations within a few (approx. 3) computational cells.

The simulated shock-tube experiments involve high (SF$_6$) and low density (air) gases initially separated by membranes and wire mesh, as indicated schematically in figure 4 for the inverse chevron configuration (Youngs 2007). We model the experimental set-up approximately as follows. The contact discontinuity between air and SF$_6$ is modelled as a jump in density using ideal gases with $\gamma=1.4$ and 1.076, respectively. Temperature changes appropriately so as to maintain a constant pressure across the initial interface. A shocked air
region is created upstream in terms of a higher-density, higher-pressure region chosen to satisfy the Rankine–Hugoniot relations for a Mach 1.26 shock. The simulations are carried out in a reference frame in which the air–SF$_6$ interfaces are initially at rest. The primary shock propagates in the $x$ direction through the contact discontinuities and reflects at the end of the simulation box on the right. BCs involve reflecting walls in the $y$ direction and periodicity in the $z$ direction. Uniform Cartesian grids were used.

A crucial issue when simulating RMI driven flows is that of modelling the insufficiently characterized contact discontinuity ICs in the experiments. Modelling strategies have used various superpositions of perturbation modes: (i) linearly combined $S+L$ modes, where $S$ is the smallest resolved wavelength deformation chosen to represent the result of pushing the membrane through the wire mesh and $L$ is the largest resolved scale of the order of a characteristic shock-tube transverse dimension (Cohen et al. 2002), (ii) non-deterministic $S+R$ modes (Hill et al. 2006), where $R$ is an added spatially random distribution, and (iii) a perturbation series expansion approach, such as that described in the following.

The IC in the inverse chevron shock-tube simulations considered here used the series approach proposed by Youngs (2007), where all modes between $S$ and $L$ are also included in an assumed material interface deformation of the form

$$\Delta x = A \sum_{n,m} [a_n \sin(2\pi n z/L) + b_n \cos(2\pi n z/L)]/[\cos(\pi m y/L)],$$

where $\{a_n, b_n\}$ are grid-point-independent randomly chosen numbers between $-1/2$ and $+1/2$ and $A$ is chosen to prescribe a selected standard deviation (s.d.) of the initial interface deformation. Particular choices used here were, s.d. = 0.16$h$ and characteristic length scales for the shortest and longest modes $S$ and $L$ were $8h$ and $80h$, respectively, where $h$ is the uniform computational mesh spacing.

Figure 5 shows representative results from our simulations in terms of instantaneous visualizations of the SF$_6$ mass density. At selected times of the figures, the primary shock has reflected off the end wall and propagated back towards the left, to within (figure 5a) and beyond the SF$_6$ region (figure 5b). The growth of the mixing layers is strongly affected by the interactions of the shocks with the material interfaces; there are distinct imprints of the initial shape and perturbations of the contact discontinuities at the early times, and significant further effects later after the mixing layers have been perturbed by both the primary reflected shock as well as by other secondary shocks. There is good qualitative agreement between visualizations from the present simulations and those available from the laboratory experiments and previous ILES based on using fairly different NFV numerics (Youngs 2007). This suggests that major features of the underlying complex non-planar shock and vortex dynamics can be robustly captured with ILES once ICs are sufficiently characterized and suitably modelled.

### 5. Concluding remarks

Accurate predictions with quantifiable uncertainty are essential to many practical turbulent flow applications exhibiting extreme geometrical complexity and broad ranges of length and time scales. Under-resolved computer studies are

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unavoidable in such applications, and LES becomes the effective simulation strategy mostly by necessity rather than by choice. We have noted the inherently intrusive nature of both computed and laboratory experiments due to their potential sensitivity to SGS and SPGS aspects, which often appear intertwined. Crucial challenges in this context are then related to identifying and modelling the unresolved SGS and SPGS features to fully characterize the flow realizations to be simulated and assessing the associated uncertainties of the LES predictions.

SGS issues have motivated intense research in the last four decades. A crucial practical computational issue is the need to distinctly separate the effects of explicit filtering and SGS reconstruction models from the unavoidable implicit ones due to discretization. ILES addresses the seemingly insurmountable issues posed to LES by under-resolution, by focusing on the use of SGS modelling and filtering provided implicitly by physics capturing numerics. ILES has been successfully applied to a broad range of free and wall-bounded flows, ranging from canonical benchmark flows to extremely complex flows at the frontiers of current flow simulation capabilities. The performance of representative LES and ILES approaches is found to be equally good in emulating physical statistics of turbulent velocity fluctuations, and there is no discriminating characteristic favouring one or another. Looking towards practical complex flows and regimes, however, the ability of ILES to offer a simpler computational environment should be clearly emphasized.

Figure 4. Configuration of the inverse chevron shock tube used by Youngs (2007).

Figure 5. Comparative visualizations of RAGE–Godunov VL-IP simulations and the Atomic Weapons Establishment (AWE) shock-tube experiments (Youngs 2007) at two selected times: (a) \( t = 1.97 \) ms and (b) \( t = 3.97 \) ms.
Depending on grid resolution and flow regimes involved, additional explicit SGS modelling may be needed with ILES to address SGS-driven flow physics, e.g. near walls and when simulating backscatter, material mixing or chemical reaction. A major research focus is on evaluating the extent to which the particular SGS physical effects can be implicitly modelled as the turbulent velocity fluctuations, recognizing when additional explicit models and/or numerical treatments are needed, and when so, addressing how to ensure that the mixed explicit and implicit SGS models effectively act in collaborative rather than interfering fashion. An important challenge in this context is that of improving MEA, the mathematical and physical framework for its analysis and development, further understanding the connections between the implicit SGS model and numerical scheme and addressing how to build SGS physics into it.

Less attention has been devoted to SPGS modelling aspects. A special focus of our discussion here has been on turbulent initial and inflow condition issues. We illustrated crucial characterization and modelling difficulties encountered when integrating LES and laboratory experiments in complex inhomogeneous flow problems of interest. The laboratory data is typically insufficiently characterized; different IC and BC choices consistent with the available information are not equivalent and can lead to significantly different flow solutions. One issue is that of having complete datasets required to close the ICs and BCs in the simulations, the other involves appropriate laboratory data acquisition and reduction to capture the relevant upwind flow physics.

SGS and SPGS modelling issues are unavoidably intertwined, as modelling difficulties due to under-resolution become compounded with the inherent sensitivity of turbulent flows to choice of ICs and BCs. Idealized fundamental problems, such as the decay of turbulence simulated in a box domain with mathematically well-defined periodic BCs, may appear to avoid confronting questions of initial and BCs. However, periodic box simulations actually involve all the difficult SGS and SPGS issues. Moreover, it has also been established that, for sufficiently long simulation times, the integral scale of turbulence will eventually saturate since the larger simulated scales cannot have unaffected growth beyond the box size, and will eventually distort the characteristic power law of the turbulence decay (Wang & George 2002; Drikakis et al. 2007).

Since nature controls the flow physics independently of SGS and SPGS constraints in the laboratory or numerical experimental process, a legitimate question to ask relates to whether instances exist for some sort of convergence of the larger scale observed flow features and dynamics, i.e. of scales much larger than characteristic numerical or instrumental resolution cut-off scales, but presumably small enough spatially and temporally, so that we can assume that they have not been heavily affected by SPGS features. Convergence issues versus resolution are typically problem dependent and very difficult to address in general. Actual values of \(Re\) characterizing the flow at the smallest resolved scales, e.g. based on the Taylor microscale, are not \textit{a priori} available in LES or ILES. Solutions associated with different resolutions are associated with correspondingly different values of some characteristic effective \(Re\); this is clearly suggested by the comparisons between ILES and DNS results in figure 1a. This is actually inherent to any LES or ILES approach, where the smallest characteristic resolved scale is determined by the resolution cut-off wavelength.
prescribed by the explicit or implicit spatial-filtering process. These issues need to get directly projected into the process of establishing suitable procedures and metrics for LES validation.

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