Prologue

Introduction to Coarse Grained Simulation

Fernando F. Grinstein

Mixing of materials by small scale turbulent motion is a critical element of many flow systems of interest in engineering, geophysics, and astrophysics. Numerical simulation plays a crucial role and turbulent mixing predictability is a major concern. Small scale resolution requirements focus typically on those of continuum fluid mechanics described by Navier–Stokes (NS) equations; different requirements are involved depending on the regime considered and on the relative importance of coupled physics such as multispecies diffusion and combustion as determined by Reynolds number (*Re*), Knudsen, Schmidt, Damköhler, and other characteristic nondimensional numbers. Direct numerical simulation (DNS), resolving *all relevant* physical space/time scales, is prohibitively expensive in the foreseeable future for most practical flows and regimes of interest at moderate-to-high *Re*. On the other end of the simulation spectrum are the Reynolds-averaged Navier–Stokes (RANS) approaches, which focus on statistical moments for an ensemble of realizations and model the turbulent effects.

Small scale turbulent flow dynamics is traditionally viewed as universal and enslaved to that of larger scales (Fig. P.1). In *coarse grained* simulation (CGS) large energy containing structures are resolved, smaller structures are spatially filtered out, and unresolved subgrid scale (SGS) effects are modeled. CGS includes classical large eddy simulation (LES) strategies [1] focusing on explicit SGS models, implicit LES (ILES) [2] relying on SGS modeling and filtering provided by *physics capturing* numerical algorithms, and more general LES using suitably mixed explicit/implicit SGS modeling. Transition to turbulence involves unsteady large scale dynamics, which can be captured by CGS but not by single-point closures typical in RANS [3]. Our fundamental views of the so-called "spectral gap" between large and small scales have significantly evolved over the past decade to provide a solid basis for the ideas of enslavement in turbulence as they relate to CGS [4]. *The CGS strategy of separating resolved/unresolved physics constitutes a viable intermediate approach between DNS and RANS to address practical geometries and multiphysics.*

As complex turbulent flow applications typically involve underresolved simulations, robustness of CGS predictions becomes the unsettled issue. If the 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 utility of CGS is questionable. The validity of the scale separation assumptions in CGS needs to be carefully tested when potentially important SGS flow physics is involved, specifically,

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Fernando F. Grinstein
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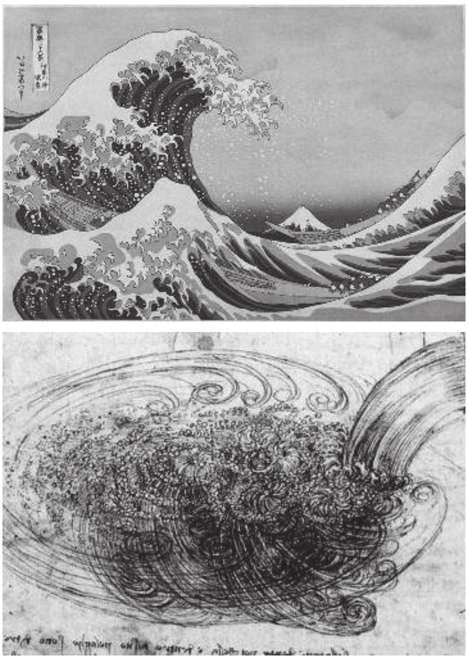

Figure P.1 Paintings by Hokusai (top) and Da Vinci (bottom) depicting universality and enslavement of small scale flow dynamics to that of large scales.

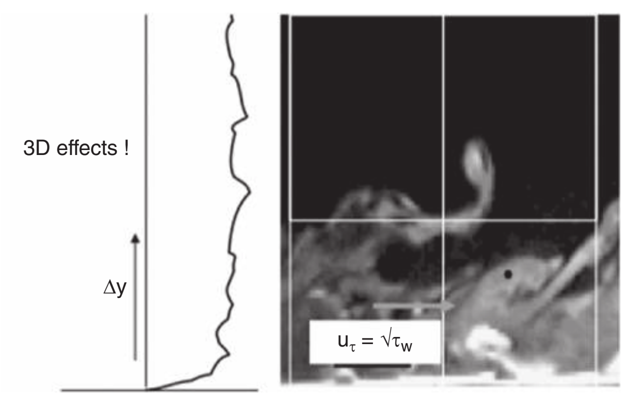

Figure P.2 Subgrid near wall features in turbulent channel flow; Δy denotes a typical CGS grid size in the direction normal to the wall, and u_τ is the inner friction velocity.

for turbulent wall bounded flows (Fig. P.2) and for turbulent material mixing (Fig. P.3) – the main focus of the book.

The book reviews our understanding of CGS of turbulent mixing, its theoretical basis, verification, validation, predictability aspects, and progress addressing difficult open issues in nonequilibrium applications involving single- as well as multiphase turbulent flow (surveyed in [5]).

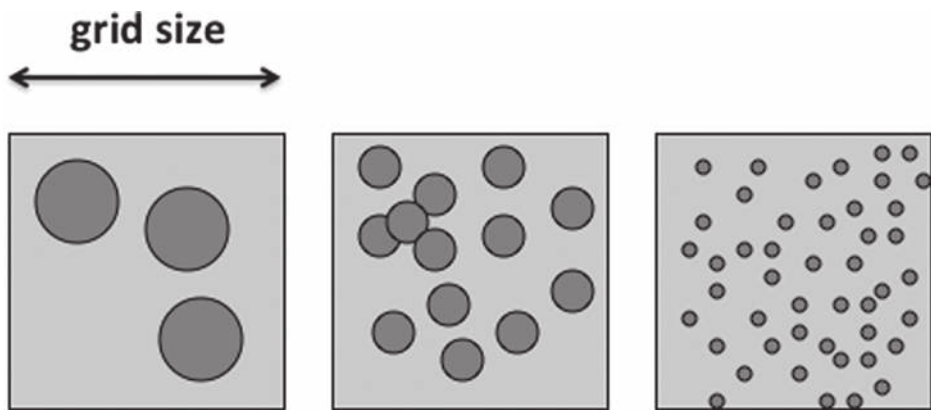

Figure P.3 Different realizations of subgrid material mixing having the same volume fractions.

P.1 CGS Fundamentals

We first address the fundamentals of the CGS paradigm: *small scales are enslaved to the dynamics of the largest*, or, put in other words, the spectral cascade rate of energy (the rate limiting step) is determined by the *initial and boundary condition constrained large scale dynamics*. The physics, computation, and metrics of enslavement and mixing for dissipative forward cascade dominated flow are introduced, and the evolution of our understanding of the role of the *spectral gap* between large (resolved) and small (modeled) scales is examined in this context.

The sensitivity of turbulent flows to initial conditions (IC) is now well recognized. Far field (late time) turbulent flows remember their particular near field (initial) features [6–9], and the mechanism by which they transition from IC to asymptotic flow occurs involves unsteady large scale coherent structure dynamics – which can be captured by CGS but not by single point closure turbulence modeling [3, 4]. The long standing view that an IC independent universal turbulence state is eventually achieved in the far field (or at late time) – for example, [10] – has been replaced by the recognition that different self-similar end states are possible depending on IC [7].

Extensive evaluations of CGS in fundamental forced and decaying isotropic homogeneous turbulence have been reported based on both Euler and NS equations [11–13]. Small scale enslavement ideas are relevant in addressing *underresolved* simulation of high-*Re* scalar mixing driven by *underresolved* velocity field in (equilibrium) isotropic forced turbulence [14, 15]. Chapter 1 shows that properly constructed CGS can be used to accurately capture [15] the dominant aspects of the mixing transition [16, 17] and established turbulent scalar mixing characteristics predicted by theory [18] and DNS [19, 20].

Chapter 2 examines fundamental ways to ensure that enough scale separation is involved in the CGS by addressing the following practical question [17]: at what flow conditions can researchers be sure that their numerical simulations have reproduced the most influential physics of the flows and fields of practical interest? Our current understanding of the energy transfer process of the turbulent flows, which forms the foundation of our scale separation arguments, is surveyed. A metric is developed using suitably available resolved tools to indicate whether the necessary physics of the flows of interest have been captured.

Finite scale theory [21], nonlinear enslavement [22], and ILES [2] all represent "top down" philosophies of modeling physical processes that rationalize a coarse grained approach to numerical simulation. Chapter 3 explores the overlap among these theories to justify and perhaps establish limits to coarse grained modeling of turbulent mixing. Finite scale equations are a coarse graining of the NS equations to describe high *Re* fluid flow. In this chapter the derivation and the properties of these equations are reviewed. The finite scale coarse graining as an extension of moment methods of kinetic theory and how the finite scale equations can be considered a hydrodynamic theory at second order are discussed. Finally an alternate explanation is proposed for physical viscosity, potentially extending the regime of the finite scale equations to length scales of the order of the molecular mean free path.

Chapter 4 examines the basics of material conservation of passive scalar mixing in finite scale NS (FSNS) fluid turbulence. Fluid motion of a NS fluid when observed at finite length and time scales is described by the equations of a second-order fluid that we call the FSNS equations. FSNS equations can also be viewed as an analytic model for ILES equations. The Reynolds averaging procedure is applied to understand the statistical fluid physics of FSNS fluid turbulence. The model problem investigated is the mixing of a passive scalar by a homogenous stationary isotropic turbulence in the presence of a mean scalar gradient. Passive scalar mixing by FSNS turbulence is shown to be mathematically consistent with the mixing fluid physics in NS turbulence, both satisfying a scalar variance conserved invariant property not exhibited by eddy viscosity models.

P.2 Challenges to Predictability

We next discuss the crucial challenges to predictability. In addition to the basic concerns regarding convergence of predictions as function of resolution, we must address the fundamental aspects of characterizing and modeling flow conditions at the SGS level – *within a computational cell or instrumentation resolution*, and at the supergrid (SPG) scale – *at initialization and boundaries of the (numerical* or *laboratory) flow experiments*. An overview of SGS and SPG issues and CGS strategies is presented, and capturing the dominant features of transition to turbulence is a particular focus.

Accurate and reliable characterization and modeling of material interfaces is an essential aspect in simulating the material mixing dynamics. Interfaces between fluids can be miscible or immiscible, with their *dynamic* character changing during evolution (and eventual phase change) of the materials. Because of SGS and SPG issues, *observations* based on numerical *or* laboratory experiments are inherently intrusive, and convergence metrics and *specific frameworks* for model verification, validation, and uncertainty quantification (VVUQ) designed *for the problems at hand* are needed to establish predictability.

Chapter 5 addresses the SGS and SPG issues. CGS strategies based on the augmented Euler or NS equations, involve the classical LES and ILES approaches. Classical LES using explicit SGS models includes many proposals ranging from simple eddy viscosity formulations to more sophisticated and accurate dynamic and mixed models [1]. Relying only on the SGS modeling and filtering provided by the numerics has been denoted numerical LES (e.g., [23]). Good or bad SGS physics can be built into the simulation model depending on the choice of numerics and its particular implementation. By sheer serendipity, physical features designed over decades into popular finite volume (FV) nonoscillatory numerical schemes to simulate shocks also provide implicit SGS models suitable for turbulent flow simulation in the ILES framework [2]. Depending on the regime of interest and grid resolution, CGS generally will involve a mixed explicit/implicit SGS strategy. Cascade pathways driven by vortex instabilities, self-induced deformations, stretching, and reconnections have been demonstrated [24, 25], and the global dynamics of transition to turbulence has been examined in terms of well-defined prototypes such as the Taylor–Green vortex [26, 27]. These processes are fundamental building blocks to be captured by CGS. Inherent to any CGS approach is the fact that the smallest characteristic resolved turbulence scale will be determined by the resolution cutoff wavelength prescribed by an explicit or implicit spatial filtering process, and practical convergence metrics must be formulated in terms of a suitable effective *Re*.

Chapter 6 examines predictability issues in multimaterial reactive flow modeling. Clouds are formed via the conversion of water vapor into cloud water or ice. This process is known as condensation, with its inverse being evaporation and the two sided process being labeled in this chapter as latent heat release. While both the time and spatial scales for latent heat release are extremely short, the integrated impact of this energy release is what drives systems such as hurricanes. Hence, when simulating systems such as hurricanes, small scales should be either resolved or represented by a SGS model; if these scales are improperly modeled, resulting predictions of intensity and track could be significantly impacted. To illustrate the impact of these numerical errors on the ability of a model to predict a system such as a hurricane, in this chapter a range of problems are presented ranging from simple advection of an isolated cloud to slightly more complex simulations of stratus clouds and finally to relatively complex simulations of hurricanes. For the two latter phenomena some of the best data sets ever obtained are compared against simulations using either traditional Eulerian or recently formulated Lagrangian cloud modeling approaches, with these comparisons revealing how differing numerical errors present in either formulation impact model predictability. Further, an aspect stressed in this chapter is how small scale processes such as evaporation can significantly influence the larger scale circulation and how numerical errors, especially those found in traditional Eulerian cloud models, make simulating this upscale energy exchange exceedingly difficult.

Chapter 7 addresses the VVUQ issues. Verification and validation are the primary means by which to assess the accuracy and reliability of numerical simulation [28].

Verification is the process of assuring that the code is solving the equations correctly, and it is usually addressed through convergence studies and analytic test problems. Validation is the process of demonstrating that one is solving the appropriate equations with the relevant SPG conditions, and is usually addressed through comparisons with available laboratory data and theoretical studies. A fundamental aspect in this context is that of assessing uncertainties in the numerical and laboratory experiments. The overall conduct of VVUQ is discussed through the construction of a relevant workflow, which by necessity is complex and hierarchical in nature. The particular characteristics of VVUQ elements depend on where the VVUQ activity takes place in the overall hierarchy of physics and models. In this chapter, the focus is on the differences between and interplay among validation, calibration, and uncertainty quantification (UQ), as well as the difference between UQ and sensitivity analysis. The complementary approach of best estimate plus reduced uncertainties approach is also discussed in some detail. The discussion is at a relatively high level; it explains the key issues associated with the overall conduct of VVUQ and offers guidance on conducting VVUQ analyses toward truly predictive turbulent mixing calculations.

P.3 Complex Mixing Consequences

Difficult challenges simulating nonequilibrium complex mixing consequences in variable density turbulent flow problems of current interest are demonstrated. For the flows discussed in this section, well-characterized whole scale laboratory studies are impossible or very difficult. Deterministic simulation studies are expensive and critically constrained by limitations in characterizing, modeling, and validating all the relevant physical subprocesses, and acquiring all the necessary and relevant SGS and SPG information. Here, we can only extrapolate from our understanding and established analysis of CGS performance in equilibrium turbulent flows, and we rely on the simulation model confidence developed from building block VVUQ and testing.

The challenging problem of underresolved mixing of material scalars promoted by underresolved velocity *and underresolved IC* in shock driven turbulent flows is examined in Chapter 8. In many areas of interest, such as inertial confinement fusion (ICF), understanding the collapse of the outer cores of supernovas, and supersonic combustion engines, vorticity is introduced at material interfaces by the impulsive loading of shock waves, and turbulence is generated via Richtmyer–Meshkov (RM) instabilities [29]. The complexity of shock waves and other compressibility effects add to the physics of material mixing, and to difficult issues of characterization and modeling of the initial and dynamic material interfaces. The inherent difficulties with the open problem of predictability of material stirring and mixing by underresolved multiscale turbulent velocity fields are now compounded with the inherent sensitivity of turbulent flows to IC [3]. The extensive recent RM simulation work [30–33] has demonstrated ILES to be an effective CGS *strategy* in this context, because of its unique combination of shock and turbulence emulation capabilities. We focus on effects of initial spectral content and interfacial morphology on transitional and late time turbulent mixing in fundamental shocktube experiments, and examine practical challenges encountered in CGS predictability evaluations in complex configurations [33] for which state of the art laboratory data and diagnostics are available.

In many noted areas of interest, such as ICF, understanding the collapse of the outer cores of supernovas, and supersonic combustion engines, vorticity is driven by the impulsive loading of shock waves and shear velocity gradients at material interfaces. In Chapter 9 we report simulations of laser driven reshock, shear, and ICF capsule experiments at the Omega laser facility [34] in the strong shock high energy density regime [35]. Validation of the simulations is based on direct comparison with radiographic data. Simulations are also compared with available DNS and theory of homogeneous isotropic turbulence. Despite the fact that the flow is neither homogeneous, isotropic, nor fully turbulent, there are local regions in which the flow demonstrates characteristics of homogeneous isotropic turbulence. We identify and isolate these regions by the presence of high levels of turbulent kinetic energy and vorticity. Our results show that in laser (shock) driven transitional flows, turbulent features such as self-similarity and isotropy only fully develop once decorrelation, characteristic vorticity distributions, and integrated turbulent kinetic energy (TKE) have decayed significantly.

Next, in Chapter 10, drive asymmetry, convergence, and the origin of turbulence in ICF implosions are examined. Uniform, spherically symmetric laser illumination of an ICF target is critical to achieving the long sought goal of high yield thermonuclear burn and gain in laser driven fusion. Unfortunately, highly symmetric laser drive of the target is extremely difficult to achieve in practice and some degree of drive asymmetry seems unavoidable. In this article we use very high resolution two- and three-dimensional numerical simulations with the LANL's RAGE code to investigate the connection between drive asymmetry and the generation of turbulence in the deuterium-tritium (DT) fuel in a simplified ICF implosion [36]. Long wavelength deviations from spherical symmetry in the pressure drive lead to the generation of coherent vortical structures in the DT gas and it is the three-dimensional instability of these structures that in turn leads to turbulence and mix. The simulations suggest that this mechanism may be an additional important source of mix in ICF implosions and may play a role in the problems being encountered at the National Ignition Facility in achieving ignition of a laser driven fusion target.

Modeling turbulent Rayleigh–Taylor driven mixing with dynamic interfaces is examined in Chapter 11. The behavior of turbulence in the presence of strong density gradients and compressibility is fundamental in applications ranging from ICF and supernovae to environmental flows. The dominant physical mechanisms at work in variable density turbulence include Kelvin–Helmholtz, Rayleigh–Taylor, and RM instabilities. All three mechanisms must be accounted for in a unified way in multiphysics simulations. Even in simplified test problems, such unstably stratified, unsteady, inhomogeneous flows pose a challenge to turbulence modeling. Rayleigh–Taylor mixing – where heavy fluid is (unstably) placed over a light fluid under the influence of gravity, is the particular focus of this chapter. Unsteady RANS have been proposed to model the mixing process across a range of complexity. Here the focus is on modeling multimaterial mixing and a dynamic interface in the tilted rig experiments, which have been studied experimentally [37] and computationally using LES [38].

Chapter 12 addresses spray combustion issues and simulation strategies in swirling flow. Nearly all flows in nature and engineering applications are turbulent and many involve complex chemical reactions. This complexity is aggravated if the flow field includes more than one phase (gas plus a liquid/solid phase) such as those encountered in gas turbine, liquid fueled rocket, and diesel engines. Combustion in such two phase flows is predominantly non-premixed, in which the heat release is controlled by the fuel–air mixing rate. Since turbulence plays an important role in increasing scalar gradients, and thus increasing mixing rates, turbulence/chemistry interaction is much more stronger in non-premixed flames compared with premixed flames. In two phase flows, the introduction of spray droplets adds several other processes with numerous time and length scales. Time scales are especially important since the liquid droplet has to vaporize and the vaporized fuel need to mix with the ambient air efficiently for combustion to occur. In order to achieve this efficiently most gas turbine combustors employ swirl as a means for aerodynamic control of spray mixing and flame holding. Prediction of spray breakdown and fuel–air mixing is critical to predict combustion efficiency in these complex systems. This chapter discusses the physics of liquid jet injection, spray formation physics, and its interaction in a swirling flow environment that is typically employed in both propulsion and power generation systems. The numerical methodologies applied to these systems are discussed along with identification of key physics critical for accurate predictions. Comparison with experimental data is used to highlight strengths and limitations of both the computational and the experimental strategies [39, 40].

Last but not least, Chapter 13 examines combustion in afterburning. Our knowledge of condensed phase explosions is limited, although explosives have existed since the gunpowder was discovered in China in the ninth century. The physical complexity of condensed phase explosions, involving extremely high pressures and temperatures, phase transitions, turbulence, shocks, mixing, instabilities, chemical reactions, and shock turbulence interactions puts very high demands on the physical modeling and the numerical simulation techniques. CGS is a cost effective approach to design full scale experiments. In enhanced blast explosives, metal particles – usually aluminum – are added to the explosive compound in order to increase the afterburning energy release by allowing the metal particles and detonation products combust with air. This presents another modeling challenge since the combustion becomes multiphased. Recent work is reviewed in the field of CGS of afterburning, including afterburning of trinitrotoluene (TNT) in unconfined air and varying the height of blast (HoB) [41], as well as multiphase afterburning of TNT/aluminum and nitromethane/steel in a spherical sector domain [42]. The main objective is to examine the use of combustion CGS to elucidate the physical processes involved in unconfined air and near ground air blasts to demonstrate effects of the HoB on afterburning and how metal particles affect combustion. The aim is to capture the most significant stages of turbulent mixing, involving the initial blast wave, secondary and reflected shocks, possible implosions, and the constant mixing stage(s), providing further knowledge of the complicated processes that occur during condensed phase explosion events.

P.4 Summary

Our present focus is on complex turbulent mixing consequences driven by variable density and compressible flow instabilities. Throughout our presentation, we emphasize the inherently intrusive nature of *coarse grained observations in computational* and *laboratory experiments*, intimately linked to their SGS and SPG specifics. Difficult challenges are then related to characterizing and modeling the unresolved SGS and SPG aspects and assessing uncertainties associated with CGS predictions and laboratory measurements. VVUQ provides the rational basis to decide when the CGS modeling is *good enough for its intended purpose*. Ensemble averaged CGS over a *suitably complete* set of realizations covering relevant IC variability is envisioned as the simulation strategy of choice to address complex flow dynamics in practical geometries.

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