Connections Between Regularized and Large-Eddy Simulation Methods for Turbulence

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1 Overview of the Field

Fluid flows are typically classified as laminar or turbulent. While the glassy, regular flow of water from a slightly opened tap is laminar, the sinuous, irregular flow of water from a fully opened tap is turbulent. In a laminar flow, the velocity and other relevant fields are deterministic functions of position and time. Photos taken at different times, no matter how far, of steady laminar flow from a tap will be identical. In a turbulent flow, the velocity and other relevant fields manifest complex spatial and temporal fluctuations. A video of steady turbulent flow from a tap will exhibit a constantly changing pattern and many length and time scales. In nature and technology, laminar flows are more the exception than the rule. Fluvial, oceanic, pyroclastic, atmospheric, and interstellar flows are generally turbulent, as are the flows of blood through the left ventricle and air in the lungs. Flows around land, sea, and air vehicles and through pipelines, heating, cooling, and ventilation systems are generally turbulent, as are most flows involved in industrial processing, combustion, chemical reactions, and crystal growth.

Turbulence enhances transport and mixing. Turbulent ocean currents can increase the encounter rate between fish larvae and their prey. Without turbulence, the fuel and air injected into the cylinder of an internal combustion engine would mix too slowly to be effective. Birds extract energy from turbulent winds to soar for great distances without flapping their wings. Turbulence can be detrimental as well. The efficiencies of vehicles, pipelines, and industrial equipment are all hindered by turbulence. Turbulence can also cause structural fatigue, generate unwanted noise, and distort the propagation of electromagnetic signals.

These observations highlight the importance of turbulence research. Our ability to predict and control turbulence and, thus, to intensify or suppress its effects as circumstances warrant is contingent on our understanding of the underlying mechanisms. Turbulence is also immensely interesting from a purely scientific perspective and is a great source of fundamentally important, challenging problems for physicists, engineers, and mathematicians. Moreover, various methods and tools developed in the field have found applications in other fields, including nonlinear optics, nonlinear acoustics, pattern formation, image processing, data compression, and econophysics.

The difficulty of achieving a physically meaningful analytical description of turbulence is well-recognized. The earliest efforts to do so, dating to works published by Boussinesq and Reynolds in the late 19th century, employed a statistical approach based upon additively splitting the flow variables entering the Navier–Stokes

(NS) equations into mean and fluctuating components. The resulting Reynolds-averaged Naver–Stokes (RANS) equations include an additional stress, the Reynolds stress, that represents all interactions between the mean flow and the turbulence. A model for these interactions closes the equations. The statistical approach provides the foundation for the RANS-based simulation methods now used extensively in commercial computational fluid dynamics codes. See Alfonsi [1] for a recent review of RANS-based methods. Although the computational cost of these methods is essentially independent of the Reynolds number, they are not without drawbacks. Most importantly, they cannot produce solutions to the NS equations. Further, since all fluctuations are averaged out, RANS-based methods cannot provide information about turbulent flow structures. They are also often found to be overly dissipative and, thus, to produce unnaturally sluggish flows. Finally, because they are based on questionable closure conditions and rely on ad hoc choices of parameters, their predictive capacity is limited.

In contrast to RANS-based simulation, direct numerical simulation (DNS) of the NS equations resolves all the eddy scales in a turbulent flow. However, for DNS of isotropic turbulence in an incompressible fluid at Reynolds number Re, memory needs and CPU usage scale with $\mathrm{Re}^{9/4}$ and Re^3, respectively. DNS simulations of realistic applications—which typically involve Reynolds numbers well in excess of 10^7—are therefore far beyond the capacity of currently available supercomputers. Even so, DNS is highly valuable from the research perspective. In particular, it provides benchmark results against which results from other methods can be compared, at moderate Reynolds numbers.

A less computationally intensive approach is provided by large eddy simulation (LES), in which a low-pass filter is used to eliminate eddy scales smaller than some width h. For LES, with filter width chosen equal to the Taylor microscale, of isotropic turbulence in an incompressible fluid, memory needs and CPU usage scale with $\mathrm{Re}^{3/2}$ and Re^2, respectively. Like averaging, filtering generates a closure problem. Interactions between the resolved and unresolved scales are accounted for by the subfilter stress arising from filtering. Closure requires an expression for the subfilter stress in terms of the resolved scales. To ensure consistency with the NS equations, this stress must become negligible as the filter width h tends to the Kolmogorov length η—the smallest dynamically relevant scale present in a turbulent flow. Although LES is now being applied to practical problems, the achievable complexity is limited by computer power, particularly in case of high-Reynolds wall-bounded flows. Even assuming that computer power continues to grow according to Moore's law, further advances in LES will hinge on developing improved subgrid models and numerical methods.

LES couples the resolution error tied to neglecting the small scales and the truncation error tied to discretization. This complicates the development of subfilter models. In an ideal LES, the net error associated with filtering and discretization will vanish when compared to filtered DNS results. Explicit LES is based first on developing subfilter models and then on constructing numerical methods that minimize the combined error. Implicit LES is based on discretization schemes in which truncation errors serve implicitly as subfilter models. While subfilter models used in explicit LES tend to be loosely motivated by statistical considerations, discretization schemes used in implicit LES are chosen for reasons of numerical expediency. Stability concerns arise for both explicit and implicit LES. Sagaut [2], Geurts [3], John [4], Berselli et al. [5], and Grinstein et al. [6] provide up-to-date descriptions and assessments of the rich spectrum of contemporary LES approaches.

It is possible, at least away from walls, to derive LES models of very high-order accuracy. However, these models also lead to correspondingly intense computational complexity for their numerical solution. Some also introduce yet more questions on the already difficult problem of specifying needed and sometimes artificial local boundary conditions for the inherently nonlocal flow averages. For these two (and other) reasons, there has been a resurgence of interest in basing simulations of turbulent flows on much simpler regularizations of the Navier–Stokes equations rather than on full models of local averages—i.e., LES models. Initially these were developed as pure theoretical tools. The influx of ideas from LES and the added constraint that the regularization be amenable to numerical simulation have breathed new ideas and thus new life into this thread of turbulence modeling.

Considerable attention is now being given to an alternative class of turbulence models that stem from direct, inviscid regularizations of the NS equations. The earliest example of such a model is the Leray [7] regularization. More recent examples include the Clark [8] model, the Bardina [9] model, the NS-α model of Chen et al. [10–12], the NS-$\alpha\beta$ model of Fried and Gurtin [13], and the NS-ω model of Layton et al. [14]. In these models, the filtered convective flux in the NS equations is modified directly. This produces regularizations that retain the many salient properties of the NS equations. For instance, Foias et al. [15] have shown that solutions to the NS-α model preserve, in an appropriately generalized sense, the circulation behavior of solutions to the NS equations and have also demonstrated that the NS-α equations possess a global attractor with finite dimension. Fried and Gurtin [13] have established Lyapunov relations for the NS-$\alpha\beta$ equations along with specializations for the NS-α equations. Global regularity results for solutions to the NS-α equations has been obtained by Foias et al. [15] and Marsden and Shkoller [16].

In a recent study of the quality of Leray, Bardina, NS-α models (along with recent modifications of the Leray and Bardina models), Geurts et al. [17, 18] showed that these regularized models can be interpreted as LES models. This exciting development indicates the potential for a useful dialog between researchers in the LES community and researchers working on mathematically-based regularizations of the NS equations.

2 Recent Developments and Open Problems

DNS is currently a highly useful research tool. Nevertheless, there is a consensus that decades might pass before computational resources become sufficient to use DNS for practical applications. Most fluid mechanicians subscribe to the belief that, in the meantime, methods that resolve the most energetically significant modes of turbulent flow at computational costs lower than DNS provide ... promising alternatives to DNS. Regularized turbulence models share common features with ...NS. Their mathematical structure provides a foundation for careful analysis. Such analysis should provide a foundation for the construction of improved LES models.

There are many significant questions that need to be addressed, including:

1. Where is the common ground between DNS and LES?
2. What are the distinguishing features of current regularized turbulence models and how do they agree with and differ from features of current LES models?
3. What general properties should regularized turbulence models possess?
4. To what extent should regularized models satisfy physical principles such as frame-indiffference and thermodynamic compatibility?
5. Is it possible to identify the subclass of regularized turbulence models that implicitly embody effective subfilter stresses?
6. For regularized turbulence models that do implicitly embody effective subfilter stresses, does the LES perspective provide insight regarding the physical nature of the underlying regularization?
7. How should boundary conditions for regularized equations such as the NS-α equation, which involves fourth order spatial derivatives, be formulated?
8. For regularized models that give rise to higher-order evolution equations, what is the meaning of the additional boundary conditions at the subfilter level in the LES context?
9. Can advanced LES approaches such as the variational multiscale model be adapted to and implemented for regularized turbulence models ?
10. To what extent should compatibility of models/regularizations and solution algorithms play a role in selection or development of LES?

3 Presentation Highlights

The proceedings began with an overview talk given by Edriss Titi, the primary message of which was that turbulence is a phenomenon that is most suitably described by long-time averages. Building toward this point, Titi discussed the distinguishing features of the Smagorinsky, Euler-α, NS-α, Euler–Voigt, NS–Voigt, and Bardina models. He also made connections with shell models and the nonlinear Schröding...er equation. Regarding flows in bounded domains, Titi described a strategy for Navier–Stokes-α equations which involves setting $\alpha = 0$ in the viscous sublayer (so that it is the NS equations that are solved there, subject to the no-slip boundary condition) and solving the NS-α equations elsewhere. Reynolds stresses calculated using this strategy are found to be in excellent agreement with those obtained from NS based simulations. When applied to pipe flow, choosing α to be 1–2$\%$ of the pipe width is found to be quite accurate. Despite its numerical feasibility, the challenges associated with establishing analytical results for this strategy are significant. This presents an important opportunity for mathematicians.

Bill Layton addressed challenges associated with the central role of legacy codes in applications-oriented simulations of turbulent flows. Most often, the inner workings of such codes are not completely understood by their users. Moreover, the developers of these codes are from generations passed and, hence, are not available for consultation. Nevertheless, many industries would face significant disruptions without these legacy codes. The objective of Layton's work on this topic is to facilitate the use of modern methods involving filtering and dealiasing in conjunction with legacy codes. To be practical, this must be achieved at low cost in both computer time and programmer effort. Importantly, the algorithms involved is so doing generate new models of turbulence and there is a strong need to understand the properties of these models, which presents an opportunity for analysis.

Bernard Geurts provided a comprehensive, unified assessment of a broad spectrum of approaches to regularizing the nonlinear convective terms entering the NS equations, with emphasis on quantifying commutation errors that accompany such regularizations. Generally, these models appear to be a bit too energetic in the small scales. Standard practice has been to compare results from simulations performed using models with results from DNS of the NS equations. However, Geurts demonstrated convincingly that it is more meaningful to compute errors relative to suitably filtered DNS data. Geurts also promoted the utility of performing tests designed to push models to their limits. In particular, Geurts showed that the Leray model is more robust than the modified Leray model.

Roel Verstappen focused on eddy-viscosity modeling within the context of LES. Based on the intuitively appealing assumption that that energy transfer should not exceed eddy dissipation, Verstappen presented an analytically-based strategy for determining the eddy viscosity with the objective of ensuring that—consistent with the insight provided in the talk of Bernard Geurts—the solution of the LES equations yields the best possible approximation of the filtered velocity field. Here, the primary objective is to reduce artifacts generated by over-damping (associated with excessively large values of the eddy viscosity). Verstappen also presented an analysis of the scale truncation properties of the regularization obtained by his approach.

Motivated by challenges associated with the modeling of volcanic eruptions, Luigi Berselli presented results based on a reduced model for suspensions of solid particles in compressible fluids. In such models, the governing equations are coupled via drag terms and a dimensionless parameter of key importance is the Stokes number, which incorporates the difference between the characteristic velocities of the air and the suspended particles. Aside from addressing the challenges associated with the effects of compressibility, Berselli's work highlights the importance of problems involving the coupling between turbulence and additional physical processes, in particular the diffusion of suspended particles.

Lars Röhe described recent advances based on the variational multiscale (VMS) method with particular emphasis on local projection stabilization (LPS). LPS is based on introducing an operator that subtracts the large scales from the symmetric part of the velocity gradient tensor. Röhe showed that, for coarsely resolved finite-element simulations of channel flow, LPS drastically reduces spurious oscillations in discrete approximations. A primary advantage of LPS stems from the symmetry of the stabilization terms. Moreover, LPS is also found to preserve the favourable stability and approximation properties of classical residual-based stabilization techniques but avoids difficulties associated with strong coupling of velocity and pressure in the stabilization terms. Röhe also discussed effective multiscale eddy viscosities and focusing boundary conditions.

Volker John brought the audience up to date on the current status of the analysis of the existence and uniqueness of solutions to the flow equations arising from regularized turbulence models and the numerical analysis of convergence properties for discretizations of those equations. A key difficulty with analyses arises due to the presence of a large constant in the Gronwall inequality. John placed special emphasis on the two-scale VMS method. He also emphasized the importance of analyzing statistics and attractors for regularized models, noting in the process that the gap between practice and theory is large and, thus, the need for increased attention to analysis. This led to the discussion of the need to design methods based on invariant measures. It was noted that although invariant measures for the NS equations exist, the physical relevance of these measures is unknown. Mathematical analysis aimed at clarifying said relevance would represent a very important advance.

Traian Illescu presented a new LES method for solving the quasigeostophic model for barotropic ocean circulation. The strategy employs a closure strategy based on approximate deconvolution. To determine the eddy viscosity, Illescu advocates matching the dissipation scale to the grid scale. Results from simulations for symmetric double-gyre wind-...driven circulation in a shallow ocean basin were presented and discussed. It was shown that approximate deconvolution captures the correct flow features on coarse meshes. A challenge, common to all quasigeostophic models, is associated with providing boundary conditions for what amounts to the (scalar) vorticity field. In the simulations described by Illescu, this field was set to zero on the boundary of the flow domain.

Jonathan Graham began by recalling a key hypothesis underlying the derivation of the NS-α model via Lagrangian averaging, namely Taylor's frozen-in turbulence hypothesis—which amounts to stipulating that the small scales advect with the large scales. As a consequence of this hypothesis, phase-locking can occur and large eddies can tumble like rigid bodies. At sufficiently low Reynolds numbers, viscous dissipation effectively "breaks-up" artificial rigid bodies. However, at sufficiently high Reynolds numbers, this is no longer the case and, due to the presence of artificial rigid bodies, the NS-α model fails to function like an LES (inasmuch as undesirably high resolutions are needed to achieve fidelity with DNS). To counteract this difficulty, Graham suggested a strategy based on filtering rigid-body motions. A method for applying this strategy to the magnetohydrodynamic NS-α equations was then described and numerical results based on that method were presented.

Hans Kuerten presented results from detailed direct numerical simulations of turbulent channel flow and compared these to LES using the Leray model. Kuerten concentrated on near-wall turbulence with focus on providing an understanding of the extent to which the model captures flow characteristics predicted by conventional DNS. Particular attention was paid to the influence of the inverse filtering operation. He showed that direct use of the Leray model for wall-bounded turbulence is not effective — more research is needed in this direction.

Leo Rebholz described studies of the impact of an adaptive nonlinear filtering on the Leray model. The method is motivated largely by the desire to avoid spurious filtering of coherent striations. This is achieved by allowing for local adjustment of the filtering operation. Rebholz described an unconditionally stable time-stepping scheme for his method. The primary advantage of this scheme is that the filtering operation is effectively linear at each time step and, thus, is decoupled from other aspects of the numerical strategy. It was, however, observed that the filtering method is not invariant with respect to Galilean changes of observer. A simple solution to this problem involves modifying the filter so that it depends not on the velocity but instead on the difference between the velocity and its filtered counterpart. Importantly, Rebholz noted that the analysis needed to establish the unconditional stability of his time-stepping scheme would go through even with this modification. A somewhat more difficult and challenging question arose in connection with the breakdown of mass balance that accompanies the proposed filtering method, leading to a very lively discussion.

Xavi Trias explored the connections between a general class of spectrally consistent regularized models for turbulent flow and DNS. He also established connections with small-large and small-small VMS models. As with the NS-α and NS-$\alpha\beta$ models, the models considered by Trias preserve the symmetry and conservation properties of the NS equations. Of particular interest is the C_4 regularization, in which the convective term in the NS equations is replaced by a fourth-order approximation involving the residual of a self-adjoint linear filter. Trias observed that the C_4 regularization yields what can be viewed as a "parameter-free" turbulence model. However, one potentially undesirable feature of the model is that it does not preserve the Galilean invariance of the NS equations. Strategies for the partial recovery of Galilean invariance were described. These involve the addition of a hyperviscous term which has the benefit of reducing spurious backscatter.

Helene Dalmann focused on establishing a sound mathematical approach to determine the suitability of any proposed turbulence model. The approach hinges on developing an appropriate error functional and, thus, an understanding of which statistics are most appropriate. In particular, Dalmann studied the properties of the eddy-viscosity based LES model of Roel Verstappen. While it was previously known that Verstappen's eddy viscosity vanishes for the 13 laminar flows previously detailed by Vr...eman, Dalmann's analysis showed that there exist other laminar flows for which Verstappen's eddy viscosity vanishes. An error functional that takes into account this additional information was presented, as were numerical results from homogeneous decaying turbulence and channel flow.

James Riley described results associated with dispersion-induced area stretching of scalar isosurfaces in turbulent flows. The surface evolution equations that emerge from these considerations relate the scalar normal velocity and curvature of the evolving surfaces and, therefore, resemble closely interfacial evolution equations from models for phase transformations. This connection suggests interesting connections with curvature-driven surface evolution equations.

Jonathan Gustafsson spoke on integral invariants that arise for homogeneous, isotropic, decaying turbulent flows of incompressible fluids. Although somewhat disjoint from the central theme of the workshop, Gustafsson's results dovetail with issues raised by Titi and others regarding invariant measures. Moreover, Gustafsson's presentation raised awareness of the importance of understanding the spatial decay properties of various correlations and of mathematical challenges associated with extending results to flows on bounded domains.

Assad Oberoi described the residual-based variational multiscale (RBVM) formulation of LES. In this formulation, a projection operator is used to separate the solution of the NS equations into coarse and fine scales. While the coarse scale equations are solved numerically, the fine scale equations are solved analytically. Specifically, an algebraic approximation for the fine scale velocities is derived wherein they are expressed in terms of the residual of the NS operator applied to the coarse scale solution. Oberai's investigations were prompted by two complementary observations. First, while the Smagorinsky model does a good job of capturing Reynolds stress transfer terms, it does not capture the cross stress transfer terms. Second, while VMS captures cross-stress transfer terms, it underpredicts Reynolds stress transfer terms. To remedy this, Obera...i adds an additional, dynamic Smagorinksy, eddy-viscosity term, leading to a mixed model capable of accurately modeling all components of the subgrid stress.

Gantumur Tsogtgerel established the well-posedness of the NS-$\alpha\beta$ equations for bounded flows. Like the NS-α equations, the NS-$\alpha\beta$ equations involve fourth-order spatial derivatives of the filtered velocity and, thus, require additional boundary conditions. For flow past a slip-free, impermeable surface, the requirement that the filtered velocity vanish at the boundary is augmented by what is called the "wall-eddy condition." This condition involves both the filtered vorticity and its gradient, along with the length scale β and the wall-eddy length ℓ. Physically, this condition accounts for the generation of vorticity in the viscous sublayer. Since the NS-α model arises on setting β to α in the NS-$\alpha\beta$ model, Tsogtgerel's results apply directly to the NS-α equations for bounded flows. A related mathematical challenge concerns flows in domains involving free surfaces.

Tae-Yeon Kim presented results from numerical simulations for the NS-$\alpha\beta$ equations, based on comparisons with DNS for the NS system. Both homogeneous, isotropic, decaying isotropic turbulence and turbulent channel flow were considered. Results concerning energy spectra and the alignment of vorticity structures were presented.

4 Scientific Progress Made

1. The balance between dispersive and dissipative models was discussed at length.

2. Dispersive models: Understanding of dispersive models as represented in the talks has advanced rapidly over the last years. A consensus on their strengths and weaknesses seems to be developing in the community.

3. Dissipative models: These had previously been considered a blunt instrument. However, the workshop presented several steps forward in selectivity that seem promising for development. No consensus will develop until these new possibilities are explored.

4. In informal discussions, many supported the idea of mixed models that are syntheses of both types.

5. In numerical tests,the behavior of the models on the standard test problems, such as channel flow, seems to be now well understood. Most surviving models produce acceptable answers on all but the coarsest grids. This could be due to the evolution of the models, to experience with the essential difficulties of benchmark problems or to both.

6. Predictability and computability of statistics is still an important open problem.

7. Other open problems noted include: wall-flow interactions, flow+ model sensitivities and how they cascade through the system, coupled NS systems and simulation of turbulence in complex flows, and the gap between problems for which precise analysis and computational testing can be done and the needs of simulation of industrial flows.

8. Several approaches of relating the averaging radius to the mesh width and the model micro scale were discussed.

9. Technical questions in the numerical analysis of LES were discussed, especially the Reynolds number dependence of the rate constant in Gronwall's inequality.

10. Many stressed that knowing when/how a model fails can be valuable information.

5 Outcome of the Meeting

There is a unanimous consensus among all participants that the workshop was successful on all grounds and, moreover, that it would be most useful to hold a follow-up meeting within 2–3 years.

Importantly, the workshop facilitated contacts between the regularized turbulence and LES communities, contacts which have already led to new collaborations. As a noteworthy example, Tae-Yeon Kim and Eliot Fried are currently working with Traian Illescu to develop a relatively inexpensive finite-element method with optimal convergence rates, based on the idea of the continuous-discontinuous Galerkin method, for the single-layer stationary quasigeostropic equations for the large scale wind-driven ocean circulation. As another example, Denis Hinz, Giulio Giusteri, and Eliot Fried are working with James Riley to analyze structure functions for homogeneous, isotropic decaying turbulence obtained using regularized turbulence models. Additionally, Tae-Yeon Kim, and Eliot Fried are working on methods for simulating turbulent flows involving suspended particles. Edriss Titi and Bernard Geurts are joining forces to extend regularization to rotation and stratification with applications in technology and in climate modeling. Particle-laden flow near walls is being pursued further by Hans Kuerten, Cees van der Geld and Bernard Geurts in a new collaboration. The issue of commutator errors on non-uniform meshes and the question how to deal with violation of conservation principles is considered by Roel Verstappen and Bernard Geurts.

Additionally, discussions during the workshop exposed a variety of fundamental questions and problems for future study, including:

1. Can we develop reliable strategies for predicting flow development and ensemble-averaged flow properties?

2. Is it possible to develop analytical techniques to improve upon error estimates that currently lead to Gronwall-type inequalities involving impractically large constants?

3. What connections can be established between solution-dependent filters and NS?

4. Can we quantify the influences of artificial dissipation on subgrid scale behavior?

5. How might we incorporate methods from uncertainty quantification to determine upper bounds on the errors that accompany any model?

6. Insofar as the inclusion of flow physics, what constitute suitable models and how can we test model suitability?

7. What are suitable numerical methods?

8. Can we develop a mathematical theory for reliability?

9. How might we begin to develop methods and algorithms to compute invariant measures in the form of probability distribution functions?

10. With increases understanding of regularization and LES models, how can we blend such models in sensible, desirable, and correct ways?
11. What considerations should be emphasized in developing cost functions to determine optimal choices of parameters such as eddy viscosities?

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