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Turbulent mixing and beyond: non-equilibrium processes from atomistic to astrophysical scales I

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Introduction

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In this Introduction, we summarize and provide a perspective on 11 articles on 'Turbulent mixing and beyond'. The papers represent the broad variety of themes of the subject, and are concerned with fundamental aspects of turbulence, mixing and non-equilibrium dynamics. While each paper deals with a specific problem, the collection gives a panoramic overview of the subject at its present state of understanding.

Volume 1 consists of papers by Wang & Peters [1] on turbulence; by Klimenko [2] on thermodynamics and mixing; by Volpert *et al.* [3] on anomalous diffusion; by Sukoriansky & Galperin [4] on analytical modelling of geophysical flows; by Bershadkii [5] on data interpretation in climate modelling; by Lozovatsky & Fernando [6] on measure for stirring efficiency in natural environments; by Majda & Gershgorin [7] on non-local diffusivity in climate variations; by Frederiksen *et al.* [8] on stochastic modelling of geophysical flows; by Shu [9] on application of high-order accurate nonlinear schemes in simulations of compressible flows; by Radtke *et al.* [10] on hybrid atomistic-continuum dynamic simulations of multi-scale kinetic problems; and by Sofieva *et al.* [11] on measurements of stellar scintillations for quantification of atmospheric turbulence. These papers represent the broad variety of themes of the 'Turbulent mixing and beyond' programme [12] and are concerned with the fundamental aspects of turbulence, mixing and non-equilibrium dynamics.

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One of the fundamental problems in turbulence is the identification of its natural representation. An adequate representation would enable the separation of the flow scale and dynamics in ways that are not only intuitive but also analytically feasible. The canonical Fourier representation, which has been successfully applied in homogeneous turbulent flows, defines wavevectors that are local in wavevector space but non-local in physical space. Thus, it has limitations in describing turbulent structures in real space. Various other mathematical tools have been suggested in the past years to capture the dynamics of turbulent structures, with each representation assuming different levels of complexity and ease of interpretation of realistic physical contexts. The paper by Wang & Peters [1] reviews various approaches to the problem of adequate representation of turbulent structures. For instance, the dissipation elements for a scalar variable can be defined by pairs of scalar extrema (each containing one maximum and one minimum); a simpler example is the definition of a streamtube of a vector field bounded by the adjacent extremal points of the velocity magnitude. In principle, statistics conditioned on the structures may build an important linkage between turbulence physics and geometry, and may provide us with a broader view and deeper insights into flow dynamics and turbulence modelling. The authors extensively discuss this point of view in their paper.

Thermodynamics occupies a special place in physical sciences because it posits irreversibility, and hence a direction for the arrow of time, as its principal law in closed systems. While the second law of thermodynamics suggests an eventual grinding down to a common equilibrium state, our experience in open systems is that the evolution towards complex forms of organization is more the norm. This interesting topic, which broadly forms the subject of non-equilibrium thermodynamics, is the theme of Klimenko's paper [2]. The author discusses the combustion problem in the form of competition between the elements of a large and complex system. This framework is now detached from the original field of mixing in turbulent reacting flows. Conventional mixing is dissipative and conservative, while competitive mixing is discriminating. The competition rules may be of transitive (in the classical mathematical meaning) or intransitive type. The author reviews Gibbs mutations, the competitive H theorem and transitive and intransitive competitions. These concepts are then tentatively applied to turbulent flows. The development and breakdown of turbulent eddies is interpreted as a competition between turbulent eddies and exchange between the Reynolds stress tensor components in shear flows, and provide an example of intransitivity in turbulence.

The next paper in the issue discusses anomalous diffusion. In classical (or normal) diffusion, the mean-square displacement of a random walk increases linearly with time. The term 'anomalous diffusion' refers to instances where the relation is nonlinear. The physical process is called 'sub-diffusive' if the variation follows a power-law exponent in time that is smaller than unity, and 'super-diffusive' otherwise. Since there are many instances of both varieties in practice as well as mathematical models, there is great interest in understanding the generic reasons for anomalous diffusion. Current explanations include continuous-time random walks, fractional Brownian motion, diffusion on fractal topology and so forth. A large part of the work involves advection–diffusion mechanisms. Including reactions in this phenomenology is an important step towards understanding anomalous diffusion in systems such as those with a reaction front separating two homogeneous subcomponents, one or both of which may be stable. In this regard, our understanding of super-diffusive systems is better than that of sub-diffusive systems. Volpert *et al.* [3] review our current knowledge of the systems with non-Gaussian diffusion processes with fronts separating otherwise homogeneous systems. The authors suggest a number of interesting applications for which the work is relevant. They range from hydrodynamics to spreading of infectious diseases. It should, however, be pointed out that diffusion in systems with shock waves or diffusion with fronts across patterns (as opposed to homogeneous subsystems) are beyond the scope of the present article.

The standard spectral theory of the inertial-range turbulence posits a $-5/3$ roll-off of the turbulent energy as a function of the wavenumber [13–15]. In stratified flows, one expects a range of larger scales, which are affected directly by buoyancy. In this so-called buoyancy subrange of stably stratified turbulence, encompassing an intermediate range of scales larger than those of the inertial subrange, the dynamics is governed by the energy exchange between waves and small-scale turbulence. Progressive anisotropization of flow characteristics occurs on increasing spatial scales. The theoretical understanding of this region is not on the same level as that of the inertial range. The article by Sukoriansky & Galperin [4] presents an investigation of the buoyancy subrange using the so-called quasi-normal scale elimination theory of turbulence. The authors show that the theory is analytically tractable in the limit of weak stratification and yields simple expressions for horizontal and vertical eddy viscosities and eddy diffusivities. Predictions of the theory are shown to agree well with the data. Furthermore, the work sheds light on the k^{-3} spectrum whose physical nature has not been fully understood.

A full appreciation of global climatology is still an unattained goal. There are essentially two mutually dependent approaches: observations and their interpretations on the one hand, and modelling and simulations on the other. Acquiring a systematic knowledge from the data is itself not an easy and straightforward process, and is often a source of controversy. Bershadskii [5] analyses existing temperature data (Antarctic ice core data for the past 400 000 years). Since a nonlinear system driven far from equilibrium can exhibit both ordered and chaotic phenomena, the author focuses on the specific nonlinear properties of the Duffing oscillator and the 'universal' role of the one-third subharmonic resonance mechanism in the generation of strong fluctuations. Bershadskii relates it to global climate and to the role of the oceanic Rossby waves in the global temperature fluctuations of the order of a year. In particular, the author shows that large fluctuations of the reconstructed temperature on the millennial time scales are dominated by the one-third subharmonic resonance, presumably tied to the effect of Earth's precession on the energy received from the Sun by the intertropical regions. These conclusions are innovative, and it is to be hoped that climatologists will regard the interpretation as helpful.

The adequate measure of the efficiency of stirring has crucial importance for understanding natural and environmental turbulent flows. A number of measures that are currently used include: the breakdown of the invariant tori, the energy dissipation rate and the scalar concentration variance. These measures are somewhat similar, but not identical, and their suitability depends on the application. The status of a suitable measure of mixing efficiency in stratified flows is even less clear (and there are conflicting notions as to whether it is constant or a variable), though it must clearly be related to the Richardson number. Lozovatsky & Fernando [6] argue that the mixing efficiency of naturally occurring stratified shear flows is given by the parameter $\gamma = R_f\,(1 - R_f)$, where R_f is the flux Richardson number. They use the wind velocity and sonic temperature data obtained near Salt Lake City, Utah, to examine the dependence of γ on both the Richardson number and the (appropriate) Reynolds number. The authors find that the mixing efficiency is a constant in certain ranges of these parameters, but not in others. Broadly speaking, the results explain the wide variability of γ noted in previous studies of geophysical problems involving turbulent mixing.

Engineering and geophysical problems involving turbulent mixing—ranging from the spread of pollutants and hazardous plumes to combustion to the effect of anthropogenic tracers in climate change—are typically very complex and it has been difficult to derive rigorous results for these complex problems. On the other hand, rigorous results can, in fact, be attained for simple models of the complex phenomena. If these models are good enough to capture qualitatively the basic ingredients of laboratory experiments and real phenomena, it is conceivable that one may better understand the underlying physical content of the observed complexity. This content could include such features as transitions between Gaussian and stretched-tail probability density functions for the passive scalar, the nature of the steady-state turbulent spectrum for scalar variance and the eddy diffusivity approximations for tracers. Such studies also advance our arsenal of mathematical tools in addressing the more difficult class of real problems. The paper by Majda & Gershgorin [7] belongs to this class and is motivated by considerations of climate variations. It develops the theme by considering the problem of zonal jets and β-plane Rossby waves. Closed exact formulas for the mean and variance of a model equation with interesting simplifications are obtained, along with results for quantities such as non-local eddy diffusivity.

Frederiksen *et al.* [8] review recent progress in the development and applications of dynamical subgrid parameterizations for geophysical flows based on statistical dynamical and stochastic methods. The focus is on approaches where the subgrid model is determined self-consistently from the statistics of closure calculations with higher resolution or from direct numerical simulations. Their approaches differ from traditional methods in that no adjustable parameters are employed in large-eddy simulations with lower resolution. The authors also briefly summarize the historical development, and the might and application of dynamical subgrid modelling in geophysical flows.

Hybrid atomistic-continuum simulation methods minimize computational cost by using the kinetic description in regions where it is needed and by treating the remainder of the computational domain via continuum methods. These schemes typically require a separation of scales to exist. This is not the case for a large class of problems, and new simulation methods are needed. Radtke *et al.* [10] consider the simulation of multi-scale kinetic problems. The approach is based on a decomposition of the kinetic description into an equilibrium part that is described analytically or numerically, and a remainder, which is described using a particle simulation method. The authors show that it is possible to derive evolution equations for the two parts from the governing kinetic equation, leading to an adaptive method. Their discussion focuses primarily on the spatial aspects of the multi-scale problem, but the authors note that multi-scales in the temporal domain can also be treated similarly. They claim that the computational cost reduction is sufficiently large to enable otherwise intractable simulations.

Spectral (or spectral-like) methods have the smallest truncation errors among the numerical schemes used in fluid dynamics. Their success, however, is conditioned on the computational domain being piecewise smooth, and their application is less valuable for computing supersonic flows where discontinuities such as shock waves are the norm. The question then is about the best alternative for handling domains with discontinuities. Shu [9] devotes his article to a review of high-order accurate weighted essentially non-oscillatory finite-difference and finite-volume schemes and the Runge–Kutta discontinuous Galerkin finite-element methods suitable for applications in compressible turbulence simulations.

The concluding paper in the volume is devoted to application of advanced experimental technologies for understanding properties of turbulence in Earth's atmosphere. Stellar scintillation, or the twinkling of the stars, is the result of interaction of stellar light with the turbulence present in the Earth's atmosphere, as first noted by Rayleigh. The article by Sofieva *et al.* [11] dwells on stellar scintillation measurements in the Earth's atmosphere and presents an overview of ground-based, air-borne and satellite measurements of stellar scintillation; it also provides an overview of the approaches to data analyses. In order to obtain the information about the Earth's atmospheric turbulence, which must be contained in observations, a solution of the inverse problem is required. Perhaps one of the most valuable applications of the turbulence parameters retrieved from the scintillation measurements is their use for optimizing various turbulence schemes at higher altitudes. The scintillation signal is also important for the parameterization of gravity wave effects in global circulation and climate models.

Turbulent mixing thus appears as a source of paradigm problems in mathematics, physics, computations, modelling and experiments. Beyond this important interdisciplinary role, it has immense consequences for a variety of physical phenomena with a broad range of applications in astrophysics, geophysics, climate, large-scale energy systems, material science, and physics of fluids and plasmas. We hope that this collection will give the readers a panoramic view of the subject, and will serve as a useful source of information on the state of the art in the field. We further hope that it will help us to integrate our knowledge on the subject and enrich its development.

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