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On Turbulence Modeling

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Abstract: A quick review is given of some methods available for turbulence modeling. The review is pessimistic about the present, optimistic about the future, and biased in favor of the author's work. The methods discussed include direct numerical simulation, moment expansions, several kinds of modeling, probability density functions, large-eddy simulation, renormalization, expansion in dominant modes, and real space renormalization based on thermal equilibrium assumptions.

Key Words: turbulence, modeling, renormalization, computation, equilibrium, vorticity

Introduction. An engineer who has to model turbulence (in particular turbulent combustion) can find thousands of papers that offer modeling strategies. These strategies are often incompatible, often very complicated and even incomprehensible, and none can be sanely viewed as both reliable and practical.

The uninitiated observer may find this situation surprising. In the last decades turbulence has attracted attention not only from engineers, but also from mathematicians, physicists, and the popular press. Every advance in chaos, fractals, dynamical systems, renormalization, as well as in the size, speed and parallelization of computers, is heralded as having solved the "turbulence problem". These claims contain some important truths. Turbulent flow is indeed chaotic, and this observation serves to justify the use of probabilistic methods. Fractals are indeed endemic to turbulence. Dynamical system theory has clarified the transition to turbulence. Renormalization is a most promising methodology. Most importantly, progress in numerical methods and the growth in computer power make

possible some remarkable calculations. Nevertheless, despite these advances, the goal of making reliable predictions in practical problems has not yet been reached.

In the next pages I shall summarize some of the methods that have been proposed for solving the prediction problem, emphasizing their conceptual bases, interconnections, and failings. Speculations about future will emerge.

First, a quick reminder of the main features of turbulence in fluids: Turbulent flow involves many scales of motion. These scales are strongly coupled, i.e., to calculate what happens on large scales, one has to take into account what happens on a broad range of small scales. However, it is generally believed that what happens on small scales is statistically independent of the large scales (how a strong coupling can coexist with statistical independence is an interesting story in itself [9]). The behavior of the small scales can conceivably be analyzed once and for all, and the problem of making predictions simplified by coupling a computed solution for large scales with a "universal" solution for small scales, a strategy related to "large-eddy simulation" (see below). Examples of "universal" results on small scales are: (i) the Kolmogorov law, which asserts that far from walls, and under appropriate conditions, the energy spectrum $E(k)$ for small but still inviscid ("inertial") scales has the form $E(k) \sim k^{-5/3}$, where k is a wave number, and (ii) the Von Karman law, which asserts that near walls, in a similar range of scales, the velocity profile has a logarithmic form.

Direct numerical simulation and large eddy simulation. Direct numerical simulation usually means a numerical solution of a problem without the added baggage of theory (I am not sure what "direct" means, and "simulation" is often used when the words "solution" or "approximation" seem presumptuous). At first glance, direct numerical simulation seems to be the way to go. The equations of motion of a fluid are known, numerical algorithms are improving rapidly, and with the growth in computer power, why be encumbered by theory?

The obvious first reason is that the range of scales that participate in most turbulent flows and that cannot be omitted is too large for handling by any computer available or planned. In order to carry out a calculation one has to reduce that range, knowingly or

through bad numerics. Such a reduction is particularly troublesome in applications to combustion, where small-scale fluctuations have an unusually large impact through the exponential dependence of Arrhenius kinetics on temperature. An intelligent reduction in the number of "degrees of freedom" requires a good understanding of the behavior of the solutions of the Navier-Stokes equations as a viscosity (numerical or physical) tends to zero — and thus a good dose of theory.

There is a subtler but equally important problem with direct simulation: The goal of a calculation is not only to produce numbers, but more significantly, to produce understanding that can pave the wave to engineering intervention. A numerical solution without theory is useless from this point of view — after all, every experiment is an analogue computation, and people have stared at experimental data for a long time without coming up with useful conclusions. In particular, theory proposes intelligent questions that a calculation can answer.

Numerical simulation should on the whole be accompanied by a theoretical framework and by conscious choices about the handling of the small scales — a mix known as "large-eddy simulation", about which more will be said below. Without such "modeling" of the small scales, numerical calculations are at present confined to the analysis of simple paradigms, i.e., relatively simple problems where the dominant mechanisms can be elucidated and the resulting understanding can possibly be incorporated into a simplified description. Some calculations of this kind are indeed extremely illuminating; well known examples include: the analysis of the effect of vortical structures in boundary layers on the Reynolds stress [4][5]; the observation of the coherent spaghetti-like vortex structures in homogeneous turbulence [22], as predicted in [6]; the observation of hairpin formation and folding mechanisms [9] that led to the theory of vortex equilibria discussed below; the recognition of the importance of pulsed jets in turbulent combustion [13].

Many numerical methods have been proposed in fluid mechanics, and this may be the place for some brief comments about them. Standard spectral methods (expansions of the form $\sum_k \mathbf{a_k} e^{i\mathbf{k}\cdot\mathbf{x}}$) have played a major role in direct numerical simulations and, indeed, were for a time synonymous with them. This has resulted from very natural historical reasons, and was prolonged by the availability of excellent spectral software; spectral methods of this

type are however intrinsically ill-suited to the description of turbulence, where localized events may be very important (more elaborate expansion methods will be commented on further below). Finite difference and finite element method seem to me to be the natural choices in most turbulence calculations; finite difference methods are flexible in the choice of differencing for different terms, in their requirement for computer algebra, and in allowing pre-existing knowledge to be built into algorithms. Finite elements are flexible in their treatment of complex geometries and in providing high-order accuracy. There exist now a variety of elegant algorithms that borrow ideas from both finite-element and finite-difference methodologies. Vortex methods, due to their intrinsically low numerical viscosity, are often very useful in revealing the essential mechanics of complicated problems. Hybrid vortex/difference or vortex/finite element methods have emerged and may be the wave of the future.

Moment expansions, the Hopf equation, pdf's, modeling. I will now start discussing methods that claim to obviate the need for resolving many scales of motion and thus to be more practical than numerical simulation. For ease of presentation, I shall start with a method that is well known to be ineffective — moment expansion with closure.

The general idea is to average the Navier-Stokes equations, in the hope that the solution of the averaged equations approximates the average solution of the true equations. The equations being nonlinear, an equation for $\langle \mathbf{u} \rangle$ ($\mathbf{u}$ = velocity, $\langle \quad \rangle$ denotes an average) involve averages of expansions quadratic in $\mathbf{u}$, the equations for expressions quadratic in $\mathbf{u}$ involve averages of expressions cubic in $\mathbf{u}$; the result is an infinite sequence of coupled equations. To obtain something solvable, one may truncate this sequence after a finite number of equations; the solutions of the truncated system are "non-realizable" after a finite time. An example of non-realizability is the following: suppose one is given two numbers, a, b, and suppose the claim is made that for some random variable η, $\langle \eta \rangle = a$, $\langle \eta^2 \rangle = b$. Note that $0 \leq \langle (\eta - \langle \eta \rangle)^2 \rangle = \langle \eta^2 \rangle - \langle \eta \rangle^2$. Unless $b - a^2 \geq 0$, there exists no random variable η for which the claim is true. Similarly, if one is given function $f_1, \ldots f_N$ with the claim that $\langle u \rangle = f_1$, $\langle u^2 \rangle = f_2$, etc., it may happen (and usually does) that the claim is non-realizable, i.e., there exists no u for which the claim is true. The reason for the

non-realizability of the results of moment closures can be dug out of the discussion of vortex equilibria below, but we shall not take the time to present the appropriate technicalities.

An interesting example that illustrates the problem of realizability has been given by Kraichnan [17]: Consider the random differential equation

$$\frac{dq(t)}{dt} = -ibq(t) , \qquad q(0) = 1 . \tag{1}$$

where b is a random variable with probability density function (pdf) $f(x)$, i.e., the probability that b is between x and $x + dx$ satisfies

$$P(x < b \leq x + dx) = f(x)dx ,$$

with $f \geq 0$, $\int f(x)dx = 1$. Equation (1) loosely resembles the equation of motion for a single Fourier mode in a spectral representation of a flow. For a given b, $q(t) = e^{ibt}$, thus

$$Q(t) = \langle q(t) \rangle = \int e^{ixt} f(x)dx ,$$

and clearly $|Q(t)| \leq Q(0) = 1$ is a realizability condition. If an averaged approximation fails to satisfy this inequality, it is not an averaged solution of (1) for any f.

Expand the solution of (1) in Taylor series, keeping the first $n + 1$ terms:

$$q_n(t) = 1 + \sum_{j=1}^{n} (-i)^j b^j t^j / j! ; \tag{2}$$

average, writing $a_j = \langle b^j \rangle$:

$$Q_n(t) = \langle q_n(t) \rangle = 1 + \sum_{j=1}^{n} (-i)^j a_j t^j / j! .$$

Clearly, $Q_n(t) \to Q(t)$, but for any finite n, even if the a_j are known *exactly*, the realizability constraint is violated for t large enough!

One can object to the relevance of this example by noting that the series (2) may be slowly convergent for large t, and that various resummations of this series can converge faster and be less susceptible to non-realizability. (For an account of resummation, or "renormalized perturbation theory", see e.g. McComb [19]; an example is $S = 1 + x + x^2 +$

$\cdots = 1 + xS$, hence $S = 1/(1-x)$.) In the context of fluid mechanics, such resummation still omits an infinite number of terms, the expansion parameter is the Reynolds number R which is near infinity, and there is no reasonable ground state around which to expand, so resummation is not likely to be of help.

People have developed moment equations that, through the addition of extra terms, guarantee the realizability of the solutions, i.e., by adding arbitrary extra terms, guarantee that the results solve *some* problem. No comment is needed.

Since chopping off a moment expansion is not a good idea, why not keep all moments? Suppose one could find a pdf for the solutions of the Navier-Stokes equations, i.e., a function that assigns probabilities to the occurrence of flows that belong to some appropriate sets; all the moments of $\mathbf{u}$ could then be determined. The pdf would be a functional, i.e., a function of an infinite number of variables (all the values that $\mathbf{u}$ can take at all the points $\mathbf{x}$ of a flow domain). Hopf [15] has indeed derived an equation that this pdf must satisfy; albeit infinite dimensional, that equation is linear. It is one of the harmful myths of turbulence theory that one should strive to solve the Hopf equation, that this job can conceivably be done and that the results would be meaningful. Suppose one had a pdf for, say, Euler incompressible flow in two or three space dimensions. Euler flows have constants of motion (circulation, impulse, helicity, etc.). They satisfy boundary conditions and, being solutions of partial differential equations, satisfy smoothness conditions. A relevant pdf must assign a zero probability to any flow that violates these constraints. This requirement is the exact analogue of the fact that, in a study of a particle system, the constants of motion must be taken into account in the formulation of a statistical theory, or else the results are wrong. The key importance of the constraints in fluid mechanics has been thoroughly demonstrated (see e.g. Chorin [9] for a review). Indeed, the exact solution that Hopf has found for his equation does not satisfy the constraints and produces an infinite mean energy at every point and velocity fields that are nowhere differentiable. The imposition of constraints on the Hopf equation makes the task of solving it at least as difficult as the task of solving the Navier-Stokes equations exactly and repeatedly so that averages can be taken.

Other pdf methods have been proposed recently for turbulence modeling, and have found

particular favor in the combustion area. The general idea is to find ordinary stochastic differential equations that model the evolution of the pdf's for the velocity field and for other variables, effectively attempting to produce a sampling procedure for solving Hopf's equation. The numerical troubles that arise in these procedures pale in comparison with their fundamental lack of soundness.

Note however that there is an *inverse* pdf method that is perfectly sound, but produces only specific numerical solutions for the Navier-Stokes equations, not sampled descriptions of their statistics: Vortex methods produce stochastic or non-stochastic ordinary differential equations, designed so that the corresponding pdf satisfy the Navier-Stokes equation.

There exist "modeling" methods, based on averaging, that do make sense. In some problems one can concentrate on the diffusive aspects of turbulence, assume that turbulent diffusion depends on local kinetic energy and scale, work out equations that embody these ideas, and sprinkle them with adjustable constants to ensure quantitative adequacy in well defined settings. For other problems, one can argue that vorticity creation and dispersal dominate the flow, and produce adjustable equations to match. When flows are well understood qualitatively and when there are good experimental data to lean on, the resulting equations can be very effective in interpolating between experiments. This is a lot, and more cannot be expected. One cannot expect to obtain a general description of turbulence that is "reduced" from the Navier-Stokes equations, in the sense that Euler's equations for a gas provide a description that is reduced from a description by Boltzmann's equation. As stated before, calculation on large scales and modeling on small scales is likely to be better than modeling alone, because then uncontrolled assumptions are applied to a smaller part of the problem.

Renormalization; expansions in dominant modes. Renormalization methods have various forms and uses in quantum and statistical physics; in the context of turbulence theory they are methods for replacing a system with many degrees of freedom by a system with fewer degrees of freedom without altering the statistics unduly.

To explain the idea, consider the problem of determining the average IQ of N people, where N is large. Suppose one can determine the IQ of a person by perusing his/her an-

swers to a list of mathematical questions. In principle, one can distribute N questionnaires to the N people, grade them, and average the result. If N is large, this may be too labor consuming.

To make life easier, divide the N people into subgroups of m, say $m = 5$, and let each subgroup work on a single questionnaire; suppose you know the ratio of the effective, apparent IQ of a group to its average IQ; call this ratio $\phi(\mathrm{IQ})$. Then grading $N/5$ questionnaires will yield the effective average IQ of the N people, and multiplication by ϕ^{-1} will get the true average.

Here is a possible shape of ϕ:

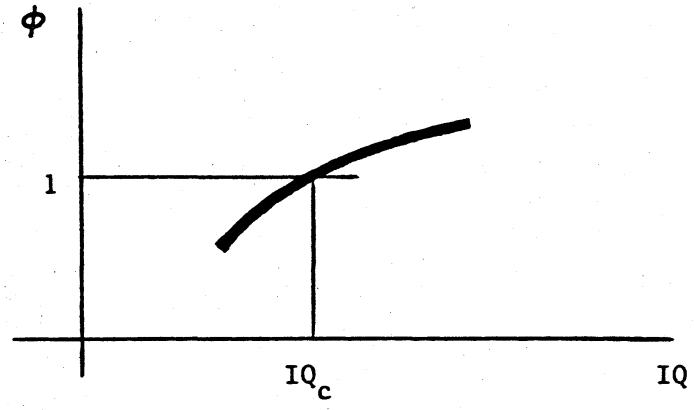

Fig. 1. Scaling function ϕ.

This shape can be rationalized as follows: smart people recognize the right answers even when they are produced by others, and a group of them is at least as smart as the smartest member of the group. Non-smart people do not accept each other's truths, and are as a group less smart than their average.

Why stop at one step of this process? Let each group of five send a representative to a committee of five such representatives, and let them decide what the answers are. One proceeds via a new level of committees rather than to groups of 25 members to ensure that the process is repetitive, and that the same ϕ can be used over and over — useful features in most applications. Assuming that the same ϕ determines the ratio of effective to average IQ for groups, one can obtain the average IQ of N people by grading $N/25$ questionnaires. This process can then be repeated, until the number of questionnaires

becomes manageable. This is a renormalization process.

Note that if IQ is less than IQ_c, the values of IQ for which $\phi = 1$, the effective IQ goes down in each iteration, until 0 is reached. If IQ > IQ_c, the effective IQ goes up. IQ=0 and IQ=∞ are stable fixed points of the renormalization. IQ=IQ_c is an unstable fixed point. At IQ=IQ_c, the average and affective IQ's are the same; such an equality should then hold for a group of people of any size, and the unstable fixed point IQ_c is then "scale invariant"; IQ_c is a "critical point". In physical systems, scale invariance occurs when the correlation length is infinite, because grouping objects into groups decreases the correlation length by shrinking the number of new objects that are correlated, except when the correlation length is infinite. When the correlation length is infinite, one expects large fluctuations and other odd phenomena.

One very effective way to carry out renormalization in physical processes is to use Fourier variables. The removal of high frequency Fourier components is a coarsening quite similar to the grouping of the IQ problem. One can take a system with wave numbers k in the range $0 < k < k_1$, do something with the ones between k_1 and $k_1 - \Delta$, Δ small, feed the information into the remaining modes and, if the new system looks like the old system with possibly new effective parameters, one can repeat the process until the number of modes is manageable. (For an expository treatment, see e.g. McComb [19].) However, what does one mean by "do something" with the unwanted modes? Some assumptions, similar to assumptions above about the shape of ϕ, must be made. One should be wary of hidden assumptions, for example assumptions to the effect that a renormalized system can still be described by a system of differential equations rather than by, for example, integro-differential equations. Much of the mathematics of this type of renormalization has been cleared up by the work of Avalleneda and Majda [2] on turbulent diffusion, where the complexity of the results, the dependence of the results on various parameters, and the dangers of hidden assumptions are explicitly apparent. One should be very wary of the application of this methodology to the full Navier-Stokes equations.

It turns out that renormalization methods can yield equations for the large scales that resemble some of the heuristic models discussed in the preceding section. This does not prove that the models are right, only that one can make assumptions both explicitly and

implicitly.

An interesting paradox appears here: one could think of getting rid of high frequency scales by renormalization, and then solve for the remaining scales by standard numerics, as in large eddy simulation. The trouble is that renormalization generally modifies the equations for the remaining scales (as in the creation of an "effective" IQ above) while large eddy simulation uses the Euler or Navier-Stokes equation for the large scales in their original state. Renormalization and large-eddy simulation reduce to each other, at least in principle, if a turbulent state is invariant under renormalization, i.e., lies at a critical point. In the next section we shall argue that is indeed so.

One may well wonder why, if renormalization is possible, is it necessary to carry it out. Why go to the trouble of creating small-scale, low energy modes and then remove them? Why not simply identify the important (e.g., energy containing) modes and forsake all others by expanding the velocity field in the few dominant modes? Such ideas have been proposed many times over the years (for an early review, see e.g. [8], for more recent attacks, see e.g. [1]). The problem is that the neglected small scales can serve as interaction catalysts and energy sinks, and cannot be neglected even if their energy is low. One can renormalize a sieve into a bowl by a proper treatment of the holes, but one cannot forget the holes and *identify* the sieve with a bowl. The energy sinks do not act uniformly on all modes, and a proper accounting for the energy loss and other features requires a good description of the dynamics of large scales, i.e., many dominant modes. (For an early analysis, see [7],[8]; for recent results, see e.g. [11].) When an expansion in dominant modes contains many terms, it becomes a special case of large-eddy simulation.

Vortex equilibria. It is increasingly recognized that turbulence, at least at low Mach numbers, is dominated by vortical structures. In other areas of physics where vortices are important, a set of renormalization methods known as "real-space renormalization", which do not use a spectral representation, have turned out to be very useful [16],[23]. This methodology can be applied to fluid dynamics [9],[10].

The first step is to construct thermal equilibria for vortex systems. In two space dimensions such equilibria have been studied by Onsager and Joyce and Montgomery, and

rigorized in recent years (for a review, see [9]). In three space dimensions such a construction has also been carried out, on a more heuristic level.

Consider a sparse collection of vortex filaments, as is appropriate for intermittent flow, and assume their lengths are fixed so that thermal equilibrium can be reached. It is enough to consider a single filament. Endow this filament with the appropriate hydrodynamical energy $E = (8\pi)^{-1} \int d\mathbf{x} \int d\mathbf{x}' \boldsymbol{\xi}(\mathbf{x}) \cdot \boldsymbol{\xi}(\mathbf{x}')/|\mathbf{x} - \mathbf{x}'|$, where $\boldsymbol{\xi}(\mathbf{x})$ is the vorticity at $\mathbf{x}$, and assign to each configuration C of the filament a Gibbs probability $P(C) \propto \exp(-E/T)$ where T is a vortex temperature that can be positive or negative. A negative temperature is "hotter" than a positive temperature, and $|T| = \infty$ is the boundary between positive and negative temperatures.

When $T < 0$ the vortex lines are smooth. When $T > 0$ vortex filaments collapse into tightly folded structures, and if reconnection is allowed, they break down into small loops. At the boundary $|T| = \infty$ the vortex lines are fractal objects whose axes has fractal dimension $\sim 5/3$; the corresponding spectrum has the Kolmogorov form. The average energy of a vortex system is an increasing function of T (remembering that $T < 0$ is hotter than $T > 0$) and of the length L of the filament. In the neighborhood of the $|T| = \infty$ transition a vortex system resembles a vortex system near the superfluid/normal fluid quantum transition, where a renormalization procedure is known.

Now suppose vortex stretching is allowed. Start with smooth vortex lines ($T < 0$). Conservation of energy and the increase in L will force the temperature down, towards $|T| = \infty$. The $|T| = \infty$ threshold is uncrossable for a continuum Euler system, and that is where such a system will remain. A viscous fluid or an underresolved numerical calculation can cross that threshold. This crossing is accompanied by a loss of energy, by reconnection, and by a growth in the fractal dimension of the filaments, and thus by excess vortex stretching and folding. (One consequence is that large energy loss and reconnection appear simultaneously.)

It goes without saying that in time-dependent problems, where the initial data are smooth and the large-scale features of the flow are time-dependent, equilibrium and quasi-equilibrium considerations apply only to the small scales of motion.

The $|T| = \infty$ turbulent state is a critical state, in the sense of the theory of critical phe-

nomena, and it shares many properties with a quantum vortex system at the temperature T_c of the superfluid transition. Indeed, in a model "$2\frac{1}{2}$ dimensional" system one can draw a curve in an appropriate parameter space that links these transitions and along which the properties of the system are invariant. It is reasonable to expect that the renormalization analysis near the superfluid transition can shed light on the turbulent state and suggest ways of "renormalizing", i.e., simplifying vortex calculations.

In a renormalization, one repeatedly removes small scales from a calculation in such a way that equilibria or dynamics are unchanged on larger scales. Assume that the small scales are in approximate thermal equilibrium, and suppose to begin with that the temperature T is finite and positive. When $T > 0$, a large vortex loop "polarizes" smaller ones, i.e., the greater likelihood of lower energies in a Gibbs distribution with $T > 0$ makes it likely that smaller loops are arranged so as to reduce the energy. The removal of small scale structures requires a decrease in vortex strength to make up for it. For $T < 0$, the opposite is true: at or near equilibrium a large loop "anti-polarizes" smaller ones, and renormalization requires the strengthening of remaining vortex lines. On the $|T| = \infty$ boundary between positive and negative temperatures one should be able to removes small loops with impunity and leave the vortex strengths invariant. The turbulent state is thus invariant under the right renormalization.

To apply this renormalization to fluid mechanics the abandonment of long cherished ideas. The universal behavior of small scales has long been explained as an essentially non-equilibrium process that moves energy from large to small scales. To apply an equilibrium theory, and the resulting recipe for handling small scales, one has to assume that though the formation of an extended spectrum is irreversible, once an inertial range is formed it lives in a neighborhood of a thermal equilibrium. In particular, energy goes up and down the ladder of scales, with a relatively small excess of energy going down over energy going up. There exists experimental evidence that supports this assumption [20]. The resulting renormalization has been tested, with positive results, only in a few simple cases [10],[21]. If this theory is valid, it opens the door to effective renormalization. It also reconciles renormalization with large eddy simulation, and explains the peculiarities of truncated moment expansions.

Conclusions. If you have to model turbulence, you have at present the following plausible options:

(i) If you have some reasonble understanding of the phenomena specific to your problem and access to some experimental data, use a simple model and keep your expectations low.

(ii) If your problem is relatively simple, if you have access to a good computer and up-to-date numerics, and if you do not need much accuracy, large-eddy simulation is surely the best option.

Major breakthroughs require new ideas, and there is hope that renormalization based on vortex equilibrium theory will provide some of them.

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List of Figure Captions

Fig. 1. Scaling function ϕ.