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Analysis of subgrid scale turbulence using the Boltzmann Bhatnagar-Gross-Krook kinetic equation

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The use of the Boltzmann kinetic equation provides a number of potential technical advantages in the analysis of subgrid scale fluid turbulence as compared to the Navier-Stokes hydrodynamic representation. The only nonlinearity in the Bhatnagar-Gross-Krook kinetic formalism occurs implicitly in the collision operator and is purely algebraic in form (even in real space). Since under Chapman-Enskog expansions one recovers the fluid equations, the alternative approach presented here should have straightforward applications to subgrid modeling of compressible turbulence and other more complex fluids. [S1063-651X(99)50803-9]

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Modern formulations of turbulence theory are based on field-theoretic methods [1,2]. A variant of this is the approach to fluid turbulence [3–5] based on the renormalization group (RG) method [6,7]. The idea is to explore scale symmetries via recursive elimination of small scales in favor of the large scales and performing scale transformations [8]. Such a procedure leads to a solution for the subgrid scale dynamics in the form of eddy dissipation. The advantage of this approach is that the local Reynolds number based on renormalized eddy viscosity can become sufficiently small to justify the use of perturbation theory [9–13]. The fundamental correctness of the RG-method remains controversial when applied to the Navier-Stokes equations [14]. Here we suggest applying the RG method at a step higher in the moment closure hierarchy.

We begin by considering the Boltzmann equation of kinetic theory,

$$\partial_t f+\mathbf{v}\cdot\nabla f=C[f], \tag{1}$$

where $f(\mathbf{x},\mathbf{v},t)$ is the probability of finding a particle in $\mathbf{x}$ at time t with velocity $\mathbf{v}$. The left-hand side represents free streaming in phase space whereas the right-hand side collects the effects of interparticle collisions. Obviously, Boltzmann equation possesses symmetry between space and time, and yet has a well defined direction of evolution indicated by an H theorem. For realistic interactions, the collision term is expressed by a very complicated integral operator [15]. The crucial point is that to all hydrodynamic purposes, including turbulence, the realistic form of the collision operator is *not* needed, simply because most details hidden in $C[f]$ play no role at the hydrodynamic level. One can therefore replace $C[f]$ with much handier expressions retaining only the basics of fluid physics. Perhaps, the simplest such model is the so-called Bhatnagar-Gross-Krook (BGK) relaxation operator [16],

$$C[f]=-\omega(f-g), \tag{2}$$

where parameter ω is an inverse characteristic relaxation time and g is a local equilibrium distribution with a Maxwellian form,

$$g=\frac{\rho}{(2\pi T)^{d/2}}\exp[-(\mathbf{v}-\mathbf{u})^2/2T], \tag{3}$$

where d is the dimension of the momentum space. It is seen that g is completely determined by the local hydrodynamic quantities, $\rho,T,$ and $\mathbf{u}$. Combination of Eqs. (1) and (2) gives the known BGK kinetic equation

$$\partial_t f+\mathbf{v}\cdot\nabla f=-\omega(f-g). \tag{4}$$

This equation is to all effects a *superset* of the Navier-Stokes equations, in the sense that the dynamics of its lower moments $\rho=\int f d^d v$, $\rho\mathbf{u}=\int f\mathbf{v}d^d v$ admits the Navier-Stokes equations in the hydrodynamic limit, defined under the Knudsen number $K_n=l_{mfp}/L\ll 1$, where $l_{mfp}\sim\sqrt{T}/\omega$ is the molecular mean free path and L is a typical scale of macroscopic interest. It is also worthwhile to point out that the BGK equation given by Eq. (4) is no longer restricted only to low density situation as opposed to the original Boltzmann equation. Since all hydrodynamic properties are contained in the BGK kinetic equation (4), theoretical analysis can be performed based on this alternative first principle description in place of the Navier-Stokes equations. At a first glance, this seems only to trouble ourselves with a lot of unwanted, redundant information from velocity space. In the recent years, mainly under the impact of lattice gas and lattice Boltzmann research, we have learned that BGK kinetic equations are amenable to simple manipulations that permit one to do away with most complexities of velocity space, including multiphase and complex boundary conditions, without corrupting the hydrodynamic content of the theory [17–20]. Boltzmann BGK given by Eq. (4) achieves the desired symmetry between space and time derivatives (hyperbolic form as opposed to mixed parabolic-hyperbolic character of the Navier-Stokes equations), and its streaming operator is lin-

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ear, which facilitates the analysis in Fourier space. Furthermore, the nonlinearity, hidden implicitly in the local Maxwellian g is entirely local in configuration space, which is another desirable technical feature. It is worth mentioning that a hyperbolic formulation of Navier-Stokes dynamics can be achieved by introducing rather complicated adjoint fields so as to couple a dissipative system with a (super)symmetric antidissipative one [21]. The elegant quasilinear form of the BGK equation provides all this in a fairly simple and natural way. This is because the aforementioned supersymmetry is just built-in in kinetic space since backward moving particles obey the adjoint version of the BGK equation for forward moving particles. Of course, at some stage the hyperbolic, symmetric form of BGK has to be broken in order to describe a dissipative system such as turbulent flows. This symmetry breaking takes place precisely at the point where the low Knudsen assumption translates into a statement of adiabatic relaxation of the (deviatoric component of) the momentum-flux tensor

$$P_{ij}=\int f v_i v_j d^d v \tag{5}$$

to its local equilibrium expression

$$P_{ij}^{eq}=\int g v_i v_j d^d v=\rho u_i u_j+\rho T\delta_{ij}.$$

This leads to the Navier-Stokes equations for a fluid with a kinematic viscosity, $\nu=T/\omega$. Conceptually, the BGK system has an intrinsic ultraviolet cutoff scale, $\sim l_{mfp}$. That is, all variations with scales less than this are viewed as thermal fluctuations, while hydrodynamic quantities such as fluid velocity $\mathbf{u}$ is nothing but the center of mass motion of the locally averaged subdomain of linear dimension l_{mfp}. From statistical physics point of view, BGK system offers a closer analogy to a spin system in which $f(\mathbf{x},\mathbf{v})$ can be conveniently compared to the density of spins at $\mathbf{x}$ associated with the state $\mathbf{v}$. This comparison is even more revealing for the lattice Boltzmann models in which the particle velocity $\mathbf{v}$ is quantized to a finite discrete set of values. Due to these mathematical features, it makes sense to explore some subgrid RG-like analysis to turbulence with the alternative kinetic representation as opposed to that for Navier-Stokes fluid equations. The resulting large scale dynamics may naturally contain a modified relaxation ω, which subsequently results in generalized transport properties involving eddy viscosity and hyperviscosities, or even the equation of state modifications. Furthermore, this alternative approach for turbulent fluid may provide a bridge over to the extensive field of knowledge in the statistical transport theory for many-body systems [22].

In what follows, we shall only present the main logical steps of the analysis together with some preliminary results. In-depth details and more rigorous treatments will be left to future presentations. To allow simpler manipulations, it is useful to start with the approximation of the Maxwellian g (an exponential non-linearity though not always undesirable) with a second order polynomial expression in the Mach number, $M\sim u/c_s(c_s^2\sim T)$,

$$g\approx\tilde{g}\equiv f_0\left[1+\frac{\mathbf{v}\cdot\mathbf{u}}{T}+\frac{(\mathbf{v}\cdot\mathbf{u})^2}{2T^2}-\frac{\mathbf{u}^2}{2T}\right], \tag{6}$$

where

$$f_0=\frac{\rho}{(2\pi T)^{d/2}}\exp[-\mathbf{v}^2/2T].$$

This is perfectly sensible as long as we restrict our attention to weakly compressible flows. Next, though arguably the advantage lies more in configuration space, in order to make an immediate comparison with existing works, we proceed with our subgrid analysis of the BGK equation in Fourier space,

$$\mathcal{S}f=-\omega(f-\tilde{g}), \tag{7}$$

where $\mathcal{S}\equiv\partial_t+i\mathbf{k}\cdot\mathbf{v}$ is a shorthand for the streaming operator and $\tilde{g}$ is the expanded local equilibrium expressed in Fourier representation. Here $f\equiv f(\mathbf{k},\mathbf{v},t)$ is the Fourier transform of the distribution function, which describes the probability density of finding a particle distribution at scale $\mathbf{k}$ having velocity value $\mathbf{v}$ at time t. It can be directly shown that the incompressible Navier-Stokes in Fourier-space results from Eq. (7) via the standard Chapman-Enskog procedure [23], together with the following explicit equilibrium form,

$$\tilde{g}=f_0\left\{\delta(\mathbf{k})+\frac{\mathbf{v}\cdot\mathbf{u}(\mathbf{k})}{T}+\left[\frac{\mathbf{G}}{2T}:\left(\frac{\mathbf{vv}}{T}-\mathbf{I}\right)\right]:\int d\mathbf{p}\mathbf{u}(\mathbf{p})\mathbf{u}(\mathbf{k}-\mathbf{p})\right\}, \tag{8}$$

where ρ and T are now pure constants, and $\mathbf{k}\cdot\mathbf{u}(\mathbf{k})=0$ in view of the incompressibility constraint. In the above, $\mathbf{I}$ is the unit tensor, and

$$\rho\mathbf{u}(\mathbf{k})=\int d^d v\,\mathbf{v}f(\mathbf{k},\mathbf{v})=\int d^d v\,\mathbf{v}\tilde{g}(\mathbf{k},\mathbf{v}).$$

The fourth-order tensor,

$$G_{ijkl}=\delta_{ik}\delta_{jl}-\delta_{ij}\frac{k_k k_l}{\mathbf{k}^2}, \tag{9}$$

is a consequence of the *total* temperature (or, pressure) change in response to maintaining incompressibility.

As we know, $l_{mfp}\equiv 2\pi/K$ defines a natural ultraviolet cutoff in wave number space, which can be set to be comparable to the Kolmogorov dissipation scale. Following the RG procedure, we can split the distribution function f into resolvable (slow) and subgrid (fast) components respectively $f=f_<+f_>$, where $f_<\equiv f(\mathbf{k},\mathbf{v};|\mathbf{k}|<K_s)$ and $f_>\equiv f(\mathbf{k},\mathbf{v};|\mathbf{k}|>K_s)$. The wave number $K_s=K/s(s\geqslant 1)$ being a new ultraviolet cutoff in Fourier space. Upon inserting this decomposition into Eq. (7), one obtains two coupled BGK equations for the resolvable and subgrid components,

$$\mathcal{S}_<f_<=-\omega(f_<-\tilde{g}_<),$$

$$\mathcal{S}_>f_>=-\omega(f_>-\tilde{g}_>), \tag{10}$$

where $\tilde{g}_< \equiv \mathcal{P}\tilde{g}$, and $\tilde{g}_> \equiv (1-\mathcal{P})\tilde{g}$ with $\mathcal{P}$ being the projector on the resolvable mode space. Manifestly, being a linear streaming operator, $\mathcal{S}$ does not introduce any coupling. The resolvable-subgrid coupling is localized to the projected equilibria $\tilde{g}_<$ and $\tilde{g}_>$. More specifically,

$$\tilde{g}_< = \tilde{g}_<^{\ll} + \delta\tilde{g}_<, \tag{11}$$

where $\tilde{g}_<^{\ll} \equiv \tilde{g}(\mathbf{u}^<)$ has the form of Eq. (8) but with the argument $\mathbf{u}$ replaced by $\mathbf{u}^< (= \int d^d v \mathbf{v} f_<)$. While $\delta\tilde{g}_< = \tilde{g}_<^{<>} + \tilde{g}_<^{\gg}$ where $<>$ and $\gg$ denote the effect on large scale equilibrium due to contributions from large-small and small-small eddy interactions, respectively. The same treatment applies to the subgrid equilibrium as well. It is often stated that a turbulent flow does *not* behave like a gas of eddies since no clear cut separation of scales can be established between fast and slow scales. This is indeed true, in that the large-small scale equilibria do *not* correspond to any local equilibrium as a function of the large-small scale flow velocity field alone, $\tilde{g}_<(\mathbf{u}) \neq \tilde{g}(\mathbf{u}^<)$. If the separation of scales were to exist and the contributions from small scales were uncorrelated random thermal-noise like fluctuations only, then the resulting hydrodynamic equation for $\mathbf{u}^<$ would be shown to be described by a trivial rescaling of the Navier-Stokes equations. In fact, because small scale properties do not generally meet with the above conditions, this rescaling is fairly nontrivial and there is no proof of such form invariance for Navier-Stokes representation [22]. On the other hand, though this remains to be shown mathematically, Eq. (7) does offer a better chance for being form invariant; a necessary requirement for a dynamical RG analysis. We can provide here a heuristic argument based on physical reasons. Supported by a local H theorem, $\tilde{g}(\mathbf{u}^<)$, corresponds to the equilibrium of a coarse grained subsystem (block spin) in a volume of size $\sim 2\pi/K_s$. Hence, we can interpret $\tilde{g}_<^{\gg}$ and $\tilde{g}_<^{<>}$ as nonequilibrium deviations from such local equilibrium caused by subgrid scale eddies. Moreover, if we argue that $\tilde{g}_<^{<>}$ can also be considered a (linear) nonequilibrium deviation, then we can formally express them, without loss of generality, as

$$\delta\tilde{g}_< = -\Delta\omega(f_< - \tilde{g}_<^{\ll}). \tag{12}$$

Substituting this into Eq. (10), we arrive at the coarse grained BGK equation,

$$\mathcal{S}_< f_< = -\tilde{\omega}(f_< - \tilde{g}_<^{\ll}). \tag{13}$$

Under these assumptions, the coarse grained BGK equation has the same form as that of the original BGK equation except with a redefined relaxation parameter (which may not necessarily be a simple scalar). Therefore, dynamic invariance at the kinetic level is more plausible. Apparently, such invariance usually does not and need not translate into a form invariance at the hydrodynamic level. Since the BGK equation reduces to the Navier-Stokes equations in the low Knudsen limit, it is clear that the new relaxation implies a modified viscosity at the $k \to 0$ limit. However, the hydrodynamic properties at some intermediate scales can become more interesting and are likely to involve not just simple eddy-damping effects.

The projected equilibrium has the following explicit form:

$$\tilde{g}_< = f_0\{\delta(\mathbf{k}) + A_i u_i^< + B_{ij}(u_i^< * u_j^< + 2u_i^< * u_j^> + u_i^> * u_j^>)\}, \tag{14}$$

where $A_i = v_i/T$, and $B_{ij} = G_{ijkl}/2T(v_k v_l/T - \delta_{kl})$, with G_{ijkl} given by Eq. (9). In the above, $u_i^< * u_j^<$ is an abbreviation for $\int d\mathbf{p} u_i^<(\mathbf{p}) u_j^<(\mathbf{k}-\mathbf{p})$. A similar definition is used for the other terms in Eq. (14). According to Eq. (11), the goal of our RG procedure is to find at each iteration of the RG analysis a sensible subgrid scale averaged expression of $\langle \delta\tilde{g}_< \rangle$ in terms of the resolvable component $f_<$ alone. Due to Eq. (10), this requires solving the small scale dynamics that is due to the resolvable-subgrid and subgrid-subgrid eddy interactions. We now make the conventional assumption that the flow carried by the subgrid component $\mathbf{u}^> = \int d^d v \mathbf{v} f_>$ splits into a high-amplitude zero-averaging component $\mathbf{u}^{>0}$ plus a low amplitude, nonzero averaging component $\mathbf{u}^{>1}$. The former is associated with a background fluctuation driven by a random force [3,9], and the latter is completely controlled by the regular motion of the large eddies. Much as in Navier-Stokes analysis, the subgrid averaged properties of these velocity fields are described as follows:

$$\langle u_i^< \rangle = u_i^<, \quad \langle u_i^{>0} \rangle = 0, \ \langle u_i^{>1} \rangle = u_i^>,$$

$$\langle u_i^{>0}(\mathbf{k}) u_j^{>0}(\mathbf{k}') \rangle = P_{ij}(\mathbf{k}) Q(k) \delta(\mathbf{k}+\mathbf{k}'), \tag{15}$$

where $P_{ij}(\mathbf{k}) \equiv \delta_{ij} - k_i k_j / k^2$ is the projection operator. Using these properties into the definition of $\langle \delta\tilde{g}_< \rangle$, we readily obtain

$$\langle \delta\tilde{g}_< \rangle = 2 f_0 B_{ij} \{u_i^< * \langle u_j^{>1} \rangle + \langle u_i^{>0} * u_j^{>1} \rangle\}. \tag{16}$$

Now we express the subgrid components via their kinetic definition, as velocity integrals of the small scale distribution function, namely $\rho u_i^{>1} = \int d^d v v_i f_>^1$, where $f_>^1$ is by definition the departure from the zeroth order subgrid local equilibrium,

$$\tilde{g}_>^0 = f_0\{A_i u_i^{>0} + B_{ij}(u_i^< * u_j^< + 2u_i^< * u_j^{>0} + u_i^{>0} * u_j^{>0})\}.$$

Though not necessary in a more systematic derivation, for the main purpose of this Rapid Communication we only consider the time variations in the subgrid mode that are short enough, so that we can ignore the time derivative in the subgrid component equation, $i\mathbf{k}\mathcal{S} \cdot \mathbf{v} \approx -(\mathbf{k} \cdot \mathbf{v})^2$. We then replace this by its ensemble averaged value and invoke isotropy, $(\mathbf{k} \cdot \mathbf{v})^2 \to \langle (\mathbf{k} \cdot \mathbf{v})^2 \rangle \to Tk^2$, then obtain to the leading order a detailed balance relation as the solution for the small scale BGK,

$$Tk^2 f_>^1 = -i\omega \mathbf{k} \cdot \mathbf{v} \tilde{g}_>^0. \tag{17}$$

Therefore, we have $f_> = (1 - i\omega\mathbf{k} \cdot \mathbf{v})\tilde{g}_>^0 + \delta f_>$, where $\delta f_>$ represents other nonequilibrium fluctuations that do not account for any hydrodynamic modes. Inserting this expression into the above velocity moment relation and using properties (15), we obtain

$$\langle u_i^{>1}(\mathbf{k})\rangle \approx \frac{-i\omega}{2Tk^2} A_{ijk}(\mathbf{k}) \int d\mathbf{p} u_j^{<}(\mathbf{p}) u^{<}{}_k(\mathbf{k}-\mathbf{p}). \quad (18)$$

Similarly, we can compute the second order moment correlation

$$\langle u_i^{>0}(\mathbf{p}) u_j^{>1}(\mathbf{k}-\mathbf{p})\rangle = \frac{-i\omega}{2Tk^2} A_{jkl}(\mathbf{k}-\mathbf{p}) u_k^{<}(\mathbf{k}) P_{il}(\mathbf{p}) Q(p). \quad (19)$$

Here, $A_{ijk}(\mathbf{k})$ is the familiar coupling kernel appearing in incompressible Navier-Stokes equations, $A_{ijk}(\mathbf{k}) = k_j P_{ik}(\mathbf{k}) + k_k P_{ij}(\mathbf{k})$ and $Q(p)$ is defined in Eq. (15). Plugging these expressions in Eq. (16), we arrive at a closed form for $\langle \delta\tilde{g}_< \rangle$ in terms of the resolvable components and averaged power spectrum of the subgrid components. The corresponding eddy viscosity is readily evaluated by either computing explicitly the contribution of $\langle \delta\tilde{g}_< \rangle$ to the momentum flux tensor in Eq. (5), or simply by inserting it into the definition of the effective relaxation $\Delta\omega$. Either way, the final result reads

$$\nu_e(k) = \frac{A_{ijk}(\mathbf{k})}{k^2} \int_> d\mathbf{p} \frac{A_{klm}(\mathbf{k}-\mathbf{p})}{\nu(\mathbf{k}-\mathbf{p})^2} P_{jl}(\mathbf{p}) P_{im}(\mathbf{k}) Q(p), \quad (20)$$

where $\nu = T/\omega$ is the molecular viscosity. This yields an effective viscosity due to scales around the cutoff K_s and represents the main result of the present Rapid Communication. Note the above expression may involve time integrations if we had not neglected the time derivative term in the subscale BGK. As in other RG procedures, we can carry on the analysis to eliminate the next wave-number shell. By so doing, the only change in expression (20) is to replace ν by $\nu_e(\mathbf{k}-\mathbf{p})$. The final result, though obtained via crude assumptions, is similar to those given by the RG derivations via Navier-Stokes representation [3,9,12]; particularly, it is identical (up to a constant factor) to that derived by Zhou and Vahala [13].

Our Boltzmann BGK-RG analysis builds upon two main assumptions: (i) the statistical properties of subgrid scales, and (ii) the low Knudsen closure. Item (i) is the same as in isotropic Navier-Stokes turbulence. On the contrary, point (ii) is peculiar to the present kinetic derivation and it has, we believe, the advantage of offering potentially new physical insights as well as alternative mathematical treatments. Nevertheless, we wish to point out that the low Knudsen assumption is not entirely rigorous, since it might become questionable in the infrared region where adiabatic enslaving to a local equilibrium is not quite accurate. More careful derivations based on systematic expansion methods are certainly warranted. This leaves room for future work which may discover additional physics besides the Navier-Stokes formulation.

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