On a New Definition of the Reynolds Number from the Interplay of Macroscopic and Microscopic Phenomenology

B.E.J. Bodmann, M.T. Vilhena, J.R. Zabadal, and D. Beck

1 Introduction

Turbulence is a behavior seen in many fluid flows, which is conjectured to be driven by the inertia to viscosity force ratio, i.e. the Reynolds number. Even though research in turbulence has existed for more than a century there is still no consensus as how to elaborate a self-consistent and genuine theory, which describes the dynamics of a transition from a laminar to a turbulent regime or vice versa, and the geometric flow structure of turbulent phenomena. So far, it is believed that the Navier–Stokes equations model turbulence in an adequate way. However the existence of general solutions in three plus one space–time dimensions is still an open question [Ca07, Ca08, Co01, Co07, Fe06].

With the present discussion we intend to take a step in a new direction and show that a connection between microscopic and macroscopic degrees of freedom may well be the crucial ingredient for progress on the subject. Usually flow phenomena are captured starting from a continuous medium fluid which, in principle, permits us to scale down volume elements to infinitesimal size. As a consequence of using an equation independent of scales implies that the laws that dictate the macroscopic dynamics do not undergo changes while altering reference lengths, or other

B.E.J. Bodmann
Universidade Federal do Rio Grande do Sul, Porto Alegre, RS, Brazil,
e-mail: bardo.bodmann@ufrgs.br

M.T. Vilhena
Universidade Federal do Rio Grande do Sul, Porto Alegre, RS, Brazil,
e-mail: vilhena@pq.cnpq.br

J.R. Zabadal
Universidade Federal do Rio Grande do Sul, Porto Alegre, RS, Brazil,
e-mail: zabadal@ufrgs.br

D. Beck
Universidade Federal do Rio Grande do Sul, Porto Alegre, RS, Brazil,
e-mail: daniel.beck@passofundo.ifsul.edu.br

C. Constanda, P.J. Harris (eds.), *Integral Methods in Science and Engineering*,
DOI 10.1007/978-0-8176-8238-5_2,

measure quantities. In fact, fluids are made from atoms and molecules which obey microscopic laws and collectively constitute a stochastic system. This system obeys macroscopic laws provided by statistical thermodynamics and hydrodynamics. Both realms can be described phenomenologically by macroscopic observables and material dependent parameters (viscosity, thermal conductivity, specific heat, compressibility, among others), where these parameters hide the microscopic properties. If one traces back the parameters until its microscopic origin, in principle it should be possible to find quantitative macroscopic-microscopic relationships beyond mere phenomenology, where viscosity and length scales among others are macroscopic manifestations with microscopic origin.

In this line we reason that turbulence, which is related to the Reynolds number, may be considered an interplay of the dynamics of at least two scales, a macroscopic one and a microscopic one. Thus, the present work is an attempt to show the possibilities that arise from, in our case, a simplified macroscopic-microscopic relationship, which we derive based on a simplified model motivated by Maxwell–Boltzmann transport. This chapter is organized as follows. In the next section we present the microscopic approach and introduce a length scale which relates to vorticity, in Sect. 3 we identify viscosity based on microscopic and thermodynamical quantities and last (Sect. 4) we discuss our findings and give future perspectives.

2 The Vortex Correlator

Consider the fluid being composed by a particle ensemble (atoms, molecules or other micro-particles), which may be characterized mechanically by a local particle density $n = n(x,y,z,t)$ and thermally by a local temperature $T = T(x,y,z,t)$. In local equilibrium one has a well defined relation between the temperature and a velocity scale $C_{th} = \sqrt{\frac{k_B T}{\langle m \rangle}}$ (the thermal velocity) where k_B is Boltzmann's constant and particles have an average mass $\langle m \rangle$. Here local equilibrium signifies that there exists a volume sufficiently small that temperature variations or equivalently variations in the velocity distribution are negligible, but that the volume contains still a sufficiently large number of particles as to represent a statistical ensemble.

Further, we assume that there exists a particle–particle interaction with associated potential, which may in general be of scalar, vector or tensor type depending on the structure of the particles under consideration and their properties. For the forthcoming discussion we assume for simplicity that the interaction may be sufficiently characterized by a scalar potential Φ. A frequently used phenomenological potential is the Lennard–Jones potential, with its large range attraction and short range repulsion [Ma81]. Once the interaction potential is known or defined, one may calculate the interaction cross section σ, the correlated mean free path $\lambda = (n\sigma)^{-1}$ and mean free propagation time $\tau_\lambda = \frac{\lambda}{C_{th}}$. To have a typical path length, below which particles in the average do not interact, makes evident the discrepancy between a continuous picture where in principle each infinitesimal volume element of the continuum influences the remainder of the fluid. The microscopic picture suggests a non-dense point set of interaction centers and a complementary dense set of interaction free points, where the microscopic behavior, because of its different topology in comparison to a continuous approach, may give rise to a different collective behavior (ensemble averages) on a macroscopic scale.

On the macroscopic scale we understand the velocity field $\vec{v}(x,y,z,t) = \langle \vec{c} \rangle$ as the ensemble average of particle velocities $\vec{c}$ in a given volume element ΔV centered at $\vec{r} = (x,y,z)$ at an instant t. The first difficulty arises when trying to capture a typical macroscopic length scale, based on a microscopic property, which shall be related to a strength with which a flow is perturbed in order to present turbulent behavior. To this end we define the dimensionless velocity vector field $\vec{G}(\vec{r},t) = \frac{\vec{v}}{C_{th}}$ and consider the field infinitesimally displaced $\vec{G} \rightarrow \vec{G}_{\delta R}$, which shall simulate the change in the velocity field by virtue of vorticity. One may establish the relation to the original field by an infinitesimal coordinate transformation, which reads

$$\begin{aligned}
\vec{G}_{\delta R}(\vec{r},t) &= \mathbf{R}\,\vec{G}(\mathbf{R}^{-1}\vec{r},t) \\
&= (1 - \delta\vec{\theta}\vec{\mathbf{G}})\,\vec{G}((1 - \delta\vec{\theta}\vec{\mathbf{G}})\vec{r},t) \\
&= \vec{G} + \delta\vec{\theta}(-\vec{\mathbf{G}}\,\vec{G} + \vec{\mathbf{G}}\,(\vec{r} \times (\vec{\nabla} \times \vec{G})))
\end{aligned}$$

where $\vec{\mathbf{G}}$ are the generators of the transformation $\mathbf{R}$ represented as a vector and each component contains a 3×3 transformation matrix which act on $\vec{G}$. $\vec{\theta}$ is the infinitesimal transformation parameter, i.e. a rotation angle with respect to a given axis $\hat{\theta}$. In component form and using the convention of summing over double indices, this reads

$$\Gamma_{\delta R\, i} = \Gamma_i + \delta\theta_j\,(-\varepsilon_{ijm}\Gamma_m + \varepsilon_{jmn} r_m \partial_n \Gamma_i) \tag{1}$$

where ε_{ijk} is the complete antisymmetric Levi-Civita symbol.

These findings may be related to vorticity using a concept from differential geometry, i.e., the generating term in (1) shall arise as a closed operator sequence—translation (Γ), vorticity (Ω), back translation and vorticity again, around a plaque of infinitesimal size.

$$\oint \Omega_i d\Gamma_j \propto -\varepsilon_{ijm}\Gamma_m + \varepsilon_{imn} r_m \partial_n \Gamma_j. \tag{2}$$

An expression compatible with (2) and for any volume of interest then has the form

$$\Omega_i = \frac{1}{V}\int_V \frac{\partial \Gamma_j}{\partial t}\,(-\varepsilon_{ijm}\Gamma_m + \varepsilon_{imn} r_m \partial_n \Gamma_j)\; d^3 r. \tag{3}$$

One identifies two contributions, an extrinsic one which explicitly depends on the position and a second contribution which is position independent and thus may have only intrinsic origin. The presence of the second term can describe vorticity without the phenomenon of creating eddies (for instance present in shear flows), whereas the first term creates eddies even for a macroscopic velocity field which derives as a gradient from a scalar potential, for which the second term cancels out. A further comment is in order here: the intrinsic term makes sense only if microscopic degrees of freedom exist that constitute the macroscopic field Γ, since it depends only on the velocity field and its temporal variation in different directions.

From this quantity (3) one may derive a macroscopic length scale which shall be used in order to define the Reynolds number. One may recognize that Ω contains the Γ fields in a bilinear form, so that the vorticity may be generalized to a correlation like function, henceforth called vorticity correlator

$$\Upsilon_t(t,t') = \frac{1}{V}\left\| \int_V \frac{\partial \Gamma_j}{\partial t}(t)\left(-\varepsilon_{ijm}\Gamma_m(t') + \varepsilon_{imn} r_m \partial_n \Gamma_j(t')\right)\, d^3r \right\| .$$

In the limit $t' \to t$ the correlator turns vorticity. Since the vorticity may be related to the angular frequency of an eddy, the correlator may be used to measure how far a particle with velocity C_{th} propagates across an eddy with non-vanishing correlations. The length scale Λ is then defined by the correlation between time and thermal velocity via the implicit relation

$$\Lambda = \tau C_{th} = \frac{C_{th}}{\sqrt{2}}\left(\left|\int_0^\tau \frac{\Upsilon_0(t,0)}{\Upsilon_t(t,0)}\, dt\right|\right)^{\frac{1}{2}} ,$$

where

$$\Upsilon_0(t,0) = \frac{1}{V}\left\| \int_V \Gamma_j(t)\left(-\varepsilon_{ijm}\Gamma_m(0) + \varepsilon_{imn} r_m \partial_n \Gamma_j(0)\right)\, d^3r \right\|$$

and the thermal noise limit $\lim_{\tau\to 0} \frac{1}{\tau}\int_0^\tau \frac{\Upsilon_0}{\Upsilon_t} dt = 2$.

So far the velocity field $\vec{v} = \langle \vec{c} \rangle$, the macroscopic length scale Λ are available from expectation values of a microscopic ensemble. The remaining quantities like the particle density and the viscosity may be determined only from an analysis of the transport equation, i.e., a Navier–Stokes type equation, which may be derived starting from the Maxwell–Boltzmann transport equation.

3 The Transport Equation

The Maxwell–Boltzmann equation describes the time evolution of the pseudo-local expectation values in a transport phenomenon. Here pseudo-local signifies local in a macroscopic (continuous) sense but discrete (by particle nature) in the microscopic sense. Its generic form is [Mu79]

$$\frac{\partial}{\partial t} n\langle \mathscr{O} \rangle + \frac{\partial}{\partial r_\mu} n\left\langle c_\mu \mathscr{O} \right\rangle - \left\langle \frac{\partial \mathscr{O}}{\partial c_\mu} b_\mu \right\rangle = n\left(\frac{\delta\langle \mathscr{O}\rangle}{\delta t}\right)_{Coll} . \qquad (4)$$

A similar equation to the Navier–Stokes one is obtained by substituting the operator to represent momentum transport $n\langle \mathscr{O} \rangle = n\left\langle mC_\mu C_\nu \right\rangle = p_{\mu\nu}$ which is also recognized as the pressure tensor; here $\vec{C} = \vec{c} - \vec{v}$. In thermal equilibrium obviously

$p_{\mu\nu} = p\delta_{\mu\nu}$ holds and since dissipative contributions are no longer at work, the diagonal (equilibrium) contributions to the pressure tensor contribute only to the homogeneous solution of the transport equation. We are interested in the dissipative part of the equation and hence reduce the pressure tensor to the friction pressure tensor

$$\pi_{\mu\nu} = nm\left\langle C_\mu C_\nu - \frac{1}{3}C^2\delta_{\mu\nu}\right\rangle$$

with zero trace $\mathscr{T}r\{\pi_{\mu\nu}\} = 0$. The second term, after decomposition and some algebraic manipulations separates a term with constant temperature and a velocity field gradient, from a term that represents heat flux, which is kinetic energy transport

$$q_\mu = \frac{n}{2}m\left\langle C^2 C_\mu\right\rangle,$$

respectively. For simplicity we ignore possible contributions of an external force field and its resulting acceleration b_μ, so that the term still to be determined is the right hand side of (4). A convenient way to simplify the equation is to approximate the collision term by an average friction pressure change

$$\frac{\delta\pi_{\mu\nu}}{\delta t} \approx \frac{\pi_{\mu\nu}}{\tau_p}$$

which renders the original equation a transport relaxation equation [Ch95, Ba08]

$$\begin{aligned}\frac{\partial}{\partial t}\pi_{\mu\nu} &+ 2nk_BT\left(\frac{1}{2}\left(\frac{\partial v_\mu}{\partial r_\nu}+\frac{\partial v_\nu}{\partial r_\mu}\right) - \frac{1}{3}\frac{\partial v_\lambda}{\partial r_\lambda}\delta_{\mu\nu}\right)\\ &+\frac{4}{5}\left(\frac{1}{2}\left(\frac{\partial q_\mu}{\partial r_\nu}+\frac{\partial q_\nu}{\partial r_\mu}\right) - \frac{1}{3}\frac{\partial q_\lambda}{\partial r_\lambda}\delta_{\mu\nu}\right) + \frac{\pi_{\mu\nu}}{\tau_p} = 0. \qquad (5)\end{aligned}$$

The relaxation time constant τ_p for phenomenological potentials and for systems not far from equilibrium in (5) may be related to the microscopic cross section in the spirit of Chapman–Cowling [Ma81]. The expression below shows the mechanical relaxation time, for an isotropic two particle interaction central potential:

$$\begin{aligned}\tau_p &= \frac{5}{16\sqrt{\pi}}\frac{1}{nC_{th}}\left(\int_0^\infty\int_0^\pi e^{-u^2}u^7(1-\cos^2(\theta))\sigma(\theta,\sqrt{2}C_{th}u)\sin(\theta)\,d\theta\,du\right)^{-1}\\ &= \frac{5}{16\sqrt{\pi}}\frac{1}{nC_{th}I_2}.\end{aligned}$$

Here u is the relative velocity between the collision partners in multiples of $\sqrt{2}C_{th}$, θ signifies the scattering angle, and C_{th} a velocity scale, i.e. the thermal velocity.

A local collision operator is responsible for the space–time evolution of the distribution in consideration. The collision term depends in general on microscopic dynamics which in many cases is not exactly known or is too complex to be evaluated analytically. However, for a number of applications there do exist interaction models [Dh07] that are sufficient to capture qualitatively as well as to a certain precision quantitatively properties of the fluid flow.

The equation above results in the Navier–Stokes type equation if the following phenomenological identity holds:

$$\pi_{\mu\nu} = -\eta_V \frac{\partial v_\lambda}{\partial r_\lambda}\delta_{\mu\nu} - 2\eta\left(\frac{1}{2}\left(\frac{\partial v_\mu}{\partial r_\nu} + \frac{\partial v_\nu}{\partial r_\mu}\right) - \frac{1}{3}\frac{\partial v_\lambda}{\partial r_\lambda}\delta_{\mu\nu}\right)$$

with η shear and η_V volumetric viscosity, respectively. By comparison one identifies the shear viscosity as

$$\eta = k_B T \tau_p = \frac{5nk_BT}{16\sqrt{\pi}C_{th}I_2} = \frac{5n\langle m\rangle C_{th}}{16\sqrt{\pi}I_2}.$$

Upon substitution of the found quantities into the traditional Reynolds number definition and replacing the usually employed macroscopic length by the vortex correlator length Λ one arrives at an expression which is characterized by two macroscopic-microscopic ratios, the correlation length Λ against the mean free path λ and the macroscopic flow velocity v against the thermal velocity C_{th} besides a factor which is determined from the collision integral and the total collision cross section σ_T.

$$\mathscr{R}e = \frac{\rho\Lambda v}{\eta} = \frac{16\sqrt{\pi}}{5}\frac{I_2}{\sigma_T}\frac{\Lambda}{\lambda}\frac{v}{C_{th}}.$$

For a collision model where the cross section $\sigma(\theta, \sqrt{2}C_{th}u)$ does not depend on the scattering angle the integral can be solved analytically and is $I_2 = \frac{\sigma_T}{\pi}$.

4 Conclusion

In the present discussion we established a connection between microscopic and macroscopic lengths and velocities which redefines the traditional Reynolds number. It is evident from its original definition that one needs a reference length in order to render the transport equation non-dimensional. In any case this length scale shall somehow synthesize the influence of boundaries and/or obstacles. Since boundaries select specific solutions from a manifold the velocity field that results from the solution of the transport equation contains this information and may thus be used to define a problem related length scale which we introduced by the vorticity correlator—a macroscopic reference length. We introduced the correlator motivated by the phenomenon that once a flow changes from laminar to turbulent flow perturbations perpendicular to the local flow velocity become important. In order to see what such a contribution looks like we analyzed the changes in the vector field under infinitesimal rotation. Making contact to the vorticity definition and generalizing our expression led to the vorticity correlator which yields only significant contributions if the afore mentioned perturbations are present in the field. These perturbations are evidently a manifestation of inner and/or outer boundaries present in the problem under consideration.

In our approach for vorticity one identifies an extrinsic (position dependent) and intrinsic contribution. The presence of the intrinsic term accounts for vorticity although the macroscopic velocity field derives from a gradient of a scalar potential, for which the curl of the extrinsic term cancels out. An intrinsic term can only be attributed to intrinsic degrees of freedom of a continuous macroscopic field and thus needs further (microscopic) degrees of freedom. In other words the macroscopic field is nothing but a macroscopic mean field from the microscopic point of view.

The counterpart to the vorticity correlator—the microscopic length—has its origin in the interpretation of the dissipation parameter (i.e. the viscosity) in terms of particle collisions which through the cross section supplies with the mean free path of the particles that constitute the fluid. At this length the scaling symmetry of macroscopic transport breaks down. It is noteworthy that these lengths may be of macroscopic magnitude (for instance they may be several *cm* in a gas). The microscopic picture for dissipation circumvents a problem that arises if the fluid in consideration behaves approximately as an ideal fluid. In the classical Reynolds definition this means that the viscosity tends to small values which rises the Reynolds number in contradiction to the fact that without dissipation turbulence will not occur. This is different from the microscopic definition where the mean free path tends to infinity (or at least is huge) which drives the Reynolds number close to zero.

A further effect comes from thermal motion in relation to the flow velocity. In a gas the thermal velocity may be orders of magnitude larger than the flow velocity, which means that the thermal noise may destroy coherent structures which are present in turbulence, because particles propagate back and forth in the fluid over lengths larger than the effective displacement length of the fluid. The closer the two velocities are the less is the influence of noise in the flow, and the formation of coherent flow patterns are possible. Such a collective behavior may not be understood from a purely macroscopic and continuous picture.

From our findings we reach a new meaning of scale invariance of the macroscopic transport equation—hydrodynamical similarity. Apart from the collision model which enters as a factor, which for a variety of interaction potentials is of the order of magnitude of 10^0, there are two relevant ratios responsible for similarity, the vorticity correlation length times the flow velocity as macroscopic expectation values compared to the mean free path times the thermal velocity, i.e. two microscopic reference quantities.

Since our considerations are an attempt to approach the turbulence problem from a microscopic-macroscopic interplay (few body interaction—collective mean field dynamics) the present discussion is a first step into a new direction. The theoretical conception presented in this work may be applied to experimental findings as for instance the visualization of the time evolution of flows and can be compared to the simulations based on the Maxwell–Boltzmann transport equation. Such an analysis is necessary to support our new definition which hopefully will prove useful in the future to classify the regimen in flows and may bring benefit for applications as for instance in the problem of dispersion of pollution in the atmosphere and water. These challenges define the next steps of future activities.

References

[Ba08] Banda, M., Klar, A., Pareschi, L., Seaïd, M.: Lattice-Boltzmann type relaxation systems and high order relaxation schemes for the incompressible Navier–Stokes equations. *Math. Comp.*, **77**, 943–965 (2008).

[Ca07] Cao, C., Titi, E.S.: Global well-posedness of the three-dimensional viscous primitive equations of large scale ocean and atmosphere dynamics. *Annals of Mathematics*, **166**, 245–267 (2007).

[Ca08] Cao, C., Titi, E.S.: Regularity criteria for the three-dimensional Navier–Stokes equations. *Indiana Univ. Math. J.*, **57**, 2643–2662 (2008).

[Ch95] Cheng, M.-C.: An efficient approach to solving the Boltzmann transport equation. *Simulation of Semiconductor Devices and Processes*, **6**, 202–205 (1995).

[Co01] Constantin, P.: Some Open Problems and Research Directions in the Mathematical Study of Fluid Dynamics. *Mathematics Unlimited and Beyond*, Springer Verlag, Berlin, 353–360 (2001).

[Co07] Constantin, P., Levant, B., Titi, E.S.: A note on the regularity of inviscid shell model of turbulence. *Physics Review E*, **75**, 016304-1–016304-10 (2007).

[Dh07] Dhama, A.K., McCourt, F.R.W., Dickinson, A.S.: Accuracy of recent potential energy surfaces for the He–N_2 interaction I: Virial and bulk transport coefficients. *J. Chem. Phys.*, **127**, 054302-1–054302-13 (2007).

[Fe06] Fefferman, C.L.: Fluids and singular integrals. *Contemporary Math.*, **411**, 39–52 (2006).

[Ma81] Maitland, G.C., Rigby, M., Smith, E.B., Wakeham,W.A.: *Intermolecular Forces: Their Origin and Determination*. Oxford University Press, Oxford (1981).

[Mu79] Muncaster, R.G.: On generating exact solutions of the Maxwell–Boltzmann equation. *Arch. Rational Mech. Anal.*, **70**, 79–90 (1979).

http://www.springer.com/978-0-8176-8237-8

Integral Methods in Science and Engineering
Computational and Analytic Aspects
Constanda, C.; Harris, P. (Eds.)
2011, XXVI, 422 p. 98 illus., Hardcover
ISBN: 978-0-8176-8237-8
A product of Birkhäuser Basel