2.1

Lecture 2.1 Kinetic molecular theory, fluid mechanics and generalized scale invariance

A quick walk through some formulae.

The mean square molecular velocity along one Cartesian coordinate is

$$\overline{v_x^2} = \sqrt{\frac{m}{2\pi k_B T}} \int_{-\infty}^{\infty} v_x^2 e^{-m v_x^2 / 2 k_B T} \, dv_x = \frac{k_B T}{m}$$

and in three dimensions the total kinetic energy of N classical particles is $3k_\mathrm{B}T/m$ where m = molecular mass and k_B is Boltzmann's constant.

One result we take from Chapman & Cowling is the **persistence of molecular velocity after collision**, their pp. 93-96 and 327. It means that **the assumption of no correlation in speed and position before and after collision with another molecule, which underlies Gaussian velocity distributions and Lorentzian line shapes in molecular spectra, is not valid.** The expression is

$$\overline{w}_{12} = \frac{1}{2} m_1 + \frac{1}{2} \frac{m_1^2}{\sqrt{m_2}} \ln\left(\frac{\sqrt{m_2} + 1}{\sqrt{m_1}} \right),$$

where $\overline{w}_{12}$ is the persistence ratio, the ratio of the mean velocity after collision to velocity before collision, m_1 is the mass of molecule 1 and m_2 is the mass of molecule 2. For equal masses, it has the value 0.406; heavy molecules take more collisions to lose their translational energy than light ones.

The central development was the invention of **molecular dynamics simulation** by numerical process on computers (Alder & Wainwright, 1970), when it was shown how fluid mechanical behaviour emerges from a population of atomic scale elastic spheres. It was discovered that when an anisotropy (in the form of a pulse of fast molecules, or a flux) was applied to an equilibrated population of Maxwellian molecules, **'ring currents'** evolved on a very short time scales (10^{-12} s) and on very small space scales (10^{-8} m). Slides 16 & 21 show the original diagram from Alder & Wainwright's paper; the 'ring current' is **hydrodynamic behaviour**, what a meteorologist would call a **vortex**. A non-equilibrium statistical mechanical explanation was provided quickly by Dorfman & Cohen (1970); they showed that the molecular velocity autocorrelation function had a 'long tail', obeying a **power law** rather than an exponential decay at long times. Quantitatively, they found that the molecular velocity correlation function, *C*, was expressible as a function of the velocity $\boldsymbol{v}(t)$ at time *t* in systems of physical dimensionality d ($d = 2 \Rightarrow$ discs; $d = 3 \Rightarrow$ spheres) by

$$C(t) = d^{-1}\langle \boldsymbol{v}(t)\cdot\boldsymbol{v}\rangle \propto t^{-d/2}.$$

Physically**, the mechanism for the emergence of the vortices is a nonlinear interaction among the faster-moving molecules**: they create high number densities ahead of themselves, leaving low number density behind. The number densities in these regions tend to equalize, creating the vortex flow**. It is a point of central importance that the energies of the fast molecules and of the vortex feed into each other – they are mutually sustaining, via positive feedback. This is a new light on the concept of vorticity, suggesting that it can emerge under anisotropy, a flux, in the simplest possible representation of a population of molecules.** It does so moreover on very short timescales, 10^{-12} seconds and on very short space scales, 10^{-8} metres; these scales are far smaller than the millimetric to centimetric scales at and below which true molecular diffusion have been traditionally considered to supplant fluid behaviour in the atmosphere.

The **vorticity form of the Navier-Stokes equation in three dimensions** [note that observationally $H_1(s) \neq 1$, where s is horizontal wind speed, so we cannot expect to view atmospheric vorticity in two dimensions and remain quantitative, since the dimensionality of atmospheric flow is $2 + H_1(s)$, see for example Schertzer and Lovejoy (1985, 1991), Tuck et al. (2004), Schertzer et al. (2012)] is

$$\frac{D\omega}{Dt} = (\boldsymbol{\omega} \cdot \nabla)\mathbf{u} + \kappa \nabla^2 \boldsymbol{\omega} \; .$$

The first term on the right says that **vorticity**, $\boldsymbol{\omega}$, **advects itself**: nonlinearity is inherent. This term alone is responsible for much of the complexity and difficulty associated with understanding, describing and computing atmospheric flow under the continuum assumption.

$\boldsymbol{\omega}$ is defined by

$$\boldsymbol{\omega} = \nabla \times \mathbf{u}$$

and by using the **autocorrelation function for vorticity**

$$\langle \boldsymbol{\omega}(t) \cdot \boldsymbol{\omega}(t) \rangle = -\nabla \langle \mathbf{u}(t) \cdot \mathbf{u}'(t) \rangle = C(t)$$

where t is time, we can define **enstrophy**:

$$\mathrm{E} = \frac{1}{2} |\boldsymbol{\omega}|^2 = 2\, C(t)$$

and enstrophy is governed by

$$\frac{D}{Dt}\left(\frac{|\boldsymbol{\omega}|^2}{2}\right) = \omega_i \omega_j S_{ij} - \kappa |\nabla \times \boldsymbol{\omega}|^2 + \nabla \cdot \left[\kappa \boldsymbol{\omega} \times (\nabla \times \boldsymbol{\omega})\right]$$

This expresses the generation of vorticity by stretching, or its destruction by compression, via the first term, balanced by viscous dissipation in the second term. The third term is the divergence, often assumed to be locally zero; this cannot be strictly true, for example, if ozone photodissociation is leading to the generation of vorticity. Here S_{ij} is the straining rate on a fluid element.

Statistical mechanics offers several **definitions of entropy. One uses vorticity**, see for example Bell and Marcus (1992). If P_l is the probability density in the l^{th} bin (grid box, cell, pixel . . .) of size δ_ω, and there are L bins all of size δ_ω, with $\omega_l = l\delta\omega$, and $l = 1, \cdots, L$,

$$P_l = \sum_{ijk} \mu(\omega_{ijk}, l)$$

where $\mu(\omega_{ijk}, l) = N^{-3}$ if $|\omega_l - \omega_{ijk}| \leq \delta_\omega / 2$ and zero otherwise.

An **entropy of the vorticity field** is then given by

$$S_w = -\sum_l P_l \ln P_l$$

(not to be confused with S_{ij} above).

We thus **can associate entropy with vorticity**, an alternative to potential temperature. Because the macroscopic definition of temperature is

$$\frac{dS}{dE} = \frac{1}{k_B T}$$

vorticity can be related to the thermodynamic state of the flow (Truesdell, 1952).

Vorticity can be normalized over an air column by dividing by the depth of the column, to yield a conservative quantity, potential vorticity (Rossby, 1940; Ertel, 1942; Hoskins et al., 1985). The full development in meteorologically familiar notation is in the last of these three references, which expounds ÔPVthinkingÕ.

For isentropic flow, using potential temperature θ - which physically is the temperature an air parcel would attain by compression if brought adiabatically to the surface - as the vertical coordinate, the absolute vorticity $(\zeta + f)$, is the sum of the relative vorticity ζ and the planetary vorticity f, so

$$\frac{d}{dt}(\zeta + f)_\theta = -(\zeta + f)_\theta \nabla_\theta \cdot \boldsymbol{v}$$

By employing the hydrostatic assumption, pressure p and θ can be related and the equation re-written as

$$\frac{d}{dt}\left\{(\zeta_\theta + f)\frac{\partial\theta}{\partial p}\right\} = 0$$

and

$$Q_\theta = (\zeta_\theta + f)\frac{\partial\theta}{\partial p}$$

expresses the potential vorticity, Q_θ.

A full quantum mechanical treatment of the atmospheric population of molecules will remain a remote fantasy for the foreseeable future, for many reasons well known in non-equilibrium statistical mechanics and also **because atmospheric molecular populations have insufficient time to achieve equilibrium distributions. This is so because the combined effects of solar flux, photochemistry, planetary rotation and gravity induce turbulent vorticity structures, with non-equilibrated, long-tailed molecular speed PDFs, on short time and space scales. There will be positive feedback between the latter and the core of jet streams, large-scale structures which can have wind speeds that are a significant fraction of the average molecular speed.**

If the density in phase space for a single molecule of mass *m*, position ***r*** and velocity ***v*** at time *t* is *f*, then Boltzmann's equation is

$$\frac{\partial f}{\partial t} + \boldsymbol{v} \cdot \nabla_r f + \frac{1}{m} \boldsymbol{F}(\boldsymbol{r}) \cdot \nabla_v f = \left(\frac{\partial f}{\partial t} \right)_{\text{collision}}, \qquad \text{(Eq. 5)}$$

where ***F***(***r***) is an external force acting on the molecule. The left hand side represents the Liouville operator expressing Hamiltonian dynamics in a potential, and is time symmetric. The right hand side is the collision integral, and even for the simplest molecular model has squared terms in *f*; for a population of molecules it also contains probabilistic expressions. The equation has lost time symmetry, a concept examined via the *H*-equation in the above references; the squared terms mean that part of the equation does not reverse sign when *t* is replaced by *-t*. Equation (5) is one of many examples of fundamental equations describing the time evolution of samples of matter which look beguilingly simple in their derivation and in their compact expression, but which nevertheless are impossibly difficult to solve analytically.

The **macroscopic relationship between vorticity and the thermodynamic state of a gas** flow was derived and investigated by Truesdell (1952), and is sometimes given in meteorological texts as the Beltrami equation (e.g. Dutton, 1986). There appears to be no microscopic equivalent, but if molecular populations behave as fluids it ought to be possible to express vorticity in terms of the molecular velocity fields via Eqs. (9 to 13) after substituting molecular velocities *v* for fluid velocities *u*. In this case,

$$\langle \omega \cdot \omega' \rangle = -\nabla \langle v \cdot v' \rangle$$

which yields **twice the enstrophy after taking the curl of the molecular velocity field**. The vorticity of ‘air’ in a molecular dynamics simulation would then arise from

$$\omega = \nabla \times v(p,q)$$

where p is molecular momentum and q is molecular position. q is necessary because the intermolecular force field for real molecules depends upon separation and angle, and because v in the atmosphere will depend upon position as a result of anisotropies arising from gravity, planetary rotation and the solar beam. In such a simulation**, the expression for the *n*th moment of the molecular speed** (Landau & Lifshitz, 1980)

$$\overline{v^n} = \frac{2}{\sqrt{\pi}}\left(\frac{2kT}{m}\right)\Gamma\left(\frac{n+3}{2}\right)$$

would allow calculation of the structure functions used in generalized scale invariance. In practice it would be necessary to investigate the averaging of the discrete molecular velocities before derivatives could be taken; it should be the minimum possible, to avoid damage to any emerging scaling properties.

Dewar's formulation says that **entropy production**, σ_Γ**, along a forward path in phase space** Γ is governed by the same, Gibbsian, distribution that Jaynes applied to the equilibrium case, namely

$$S_\Gamma = -\sum\nolimits_\Gamma p_\Gamma \ln p_\Gamma ,$$

where S_Γ is equal to the logarithm of number of phase space paths Γ with probability p_Γ, where

$$p_\Gamma \propto \exp\left(\frac{\tau\sigma_\Gamma}{2k_B}\right)$$

Instead of counting microstates as in the equilibrium case, **paths are counted in phase space for the non-equilibrium case**. From microscopic reversibility the dynamical equations are time-reversible (the dynamical equations are time-symmetric), replacement of Γ by its reversal Γ_R will result in $\sigma_{\Gamma_R} = -\sigma_\Gamma$, so

$$p_{\Gamma_R} = \exp\left(-\frac{\tau\sigma_\Gamma}{2k_B}\right)$$

from which it follows that the ratio of the probability of the forward path to that of the reversed path is

$$\frac{p_\Gamma}{p_{\Gamma_R}} = \exp\left(\frac{\tau\sigma_\Gamma}{k_B}\right)$$

This states that **the probability of the forward path Γ is exponentially greater than that of the reverse path Γ_R, a proposition that is also truer the longer is the time** τ. Violations of the second law of thermodynamics are possible in fluctuations, but not for long or over a big phase space volume, since entropy is extensive.

The **stable, random non-Gaussian processes** considered by Lévy produce probability density functions characterized by $S_\alpha(\sigma, \beta, \mu)$ where α is the stability index we have used in our formulation of generalized scale invariance, σ is scale factor (standard deviation for a Gaussian), β is skewness and μ is the mean (Samorodinsky and Taqqu, 1994). There are **only 3 known cases** that can be stated in closed form:

Gaussian: $S_2(\sigma, \beta, \mu)$ with probability density $\dfrac{1}{2\sigma\sqrt{\pi}}\exp\left(-\dfrac{(x-\mu)^2}{4\sigma^2}\right)$,

Cauchy: $S_1(\sigma, \beta, \mu)$ with probability density $\dfrac{\sigma}{\pi\left((x-\mu)^2+\sigma^2\right)}$,

Lévy: $S_{1/2}(\sigma, \beta, \mu)$ with probability density $\sqrt{\dfrac{\sigma}{2\pi}}\dfrac{1}{(x-\mu)^{3/2}}\exp\left(-\dfrac{\sigma}{2(x-\mu)}\right)$.

For $S_\alpha(\sigma, \beta, \mu)$ the upper and lower tails of the PDFs decrease like a power function. The rate of fall-off depends on α, the smaller is α the slower is the decay and the fatter is the tail. **When $\alpha < 2$ the distributions have infinite variance and when α Š 1 the mean is infinite too. Fortunately we know empirically that for atmospheric variables $1 < \alpha < 2$.** The full set of conditions governing $S_\alpha(\sigma, \beta, \mu)$ is $\alpha \in [0,2]$, σ³ 0 , $\beta \in [-1,1]$ and $\mu \in \mathbf{R}^1$. β is definable in terms of statistical moments as $\left|\Delta x^3\right| / \left|\langle \Delta x\rangle^2\right|^{3/2}$, the skewness.

It is not immediately clear how to relate H_1 and C_1 from generalized scale invariance to σ, β and μ. But we know α Å 1.6 for our atmospheric data, and we can calculate σ, β and μ. **The atmosphere qualifies as a non-Gaussian, Lévy stable random process.** In turn this has implications for prediction and numerical modelling; Gaussians may not be useful, while intermittency and multifractality have to be recognized.

The calculation procedure for H ,C_1 and α is as follows. **The quantity H_1 is the scaling exponent** calculated from an aircraft or dropsonde time series $f(t)$ by application of the first order structure function. **The q^{th} order structure function** of $f(t)$ is defined by

$$S_q(r;f) = \left\langle \left| f(t+r) - f(t) \right|^q \right\rangle$$

Where the lag r is real and positive, the angle brackets denote an average over t and ensemble averaging over f.

If a plot of log $S_q(r;f)$ versus log(r) is linear (the 95% confidence interval of the fit to obtain the slope $\zeta(q)$ is generally less than 10%), **then $\zeta(q)$ is a scaling exponent for $f(t)$.** In general we find:

$$\zeta(q) = qH - K(q)$$

where $K(q)$ characterizes the intermittency. If the intermittency is linear (of the form $K(q) = C_1(q-1)$, **C_1 is the codimension of the mean characterizing the intermittency intensity**) then the intermittency is monofractal; generally, it will be nonlinear, hence multifractal.
We then define

$$H_q = \zeta(q)/q$$

If H_q is constant as q changes, and if $K(q) = 0$,

$$\varepsilon(r,t) = \frac{1}{r}\sum_{j=t}^{t+r-1}\varepsilon(1,j), \qquad t = 1,2,3,\ldots t_{\max} - r$$

For our signals, it is found that the quantity $\left\langle \varepsilon(r,t)^q \right\rangle$ has a power law dependence on the scale r. **An unweighted linear least squares fit to** $\log\left\langle \varepsilon(r,t)^q \right\rangle$ **versus log *r* provides a slope** $-K(q)$**. A plot of** $K(q)$ **versus *q* shows a convex function with** $K(0) = K(1) = 0$**. The exponent *C*$_1$ is defined as** $K'(1)$**, evaluated here numerically from the slope defined by the points** $(0.9, K(0.9))$ **and** $(1.1, K(1.1))$**.** The uncertainty estimate in C_1 is obtained by taking the square root of the sum of the squares of the 95% confidence intervals returned by the unweighted linear least squares fits corresponding to $q = 0.9$ and $q = 1.1$. Further discussion of these procedures can be found in Schertzer and Lovejoy (1991), Tuck *et al.*, (2004) and Tuck (2008).

The multifractality index α **has the range** $0 \le \alpha \le 2$ **theoretically** and characterizes the generator of the intermittency which is the logarithm of the turbulent flux. **It may exceed 2 for data from real systems.** The corresponding fluctuations will be roughly log-Lévy except for the extreme probability tail which will generally be of a power law form with exponent q_D. Unlike Lévy variables whose probability tail has an exponent $q_D = \alpha < 2$, for the fluctuations there is no restriction on the value of q_D (note that the Gaussian is the exceptional $\alpha = 2$ case with exponential fall-off). Schertzer and Lovejoy (1991) discuss the five main cases for α; here we note that the variables we have measured appear to have $1 < \alpha < 2$ (Tuck *et al.* 2002, 2004). **Our experience indicates that a large quantity of high quality data is necessary for an accurate computation of** α**.** We use the double trace moment technique to compute α. Define

$$\varepsilon(1,\eta,t) = \frac{\left| f(t+1) - f(t) \right|^{\eta}}{\left\langle \left| f(t+1) - f(t) \right|^{\eta} \right\rangle}, \qquad t = 1,2,3,\ldots t_{\max}$$

$$\varepsilon(r,\eta,t) = \frac{1}{r}\sum_{j=t}^{t+r-1}\varepsilon(1,\eta,j), \qquad t = 1,2,3,\ldots t_{\max} - r$$

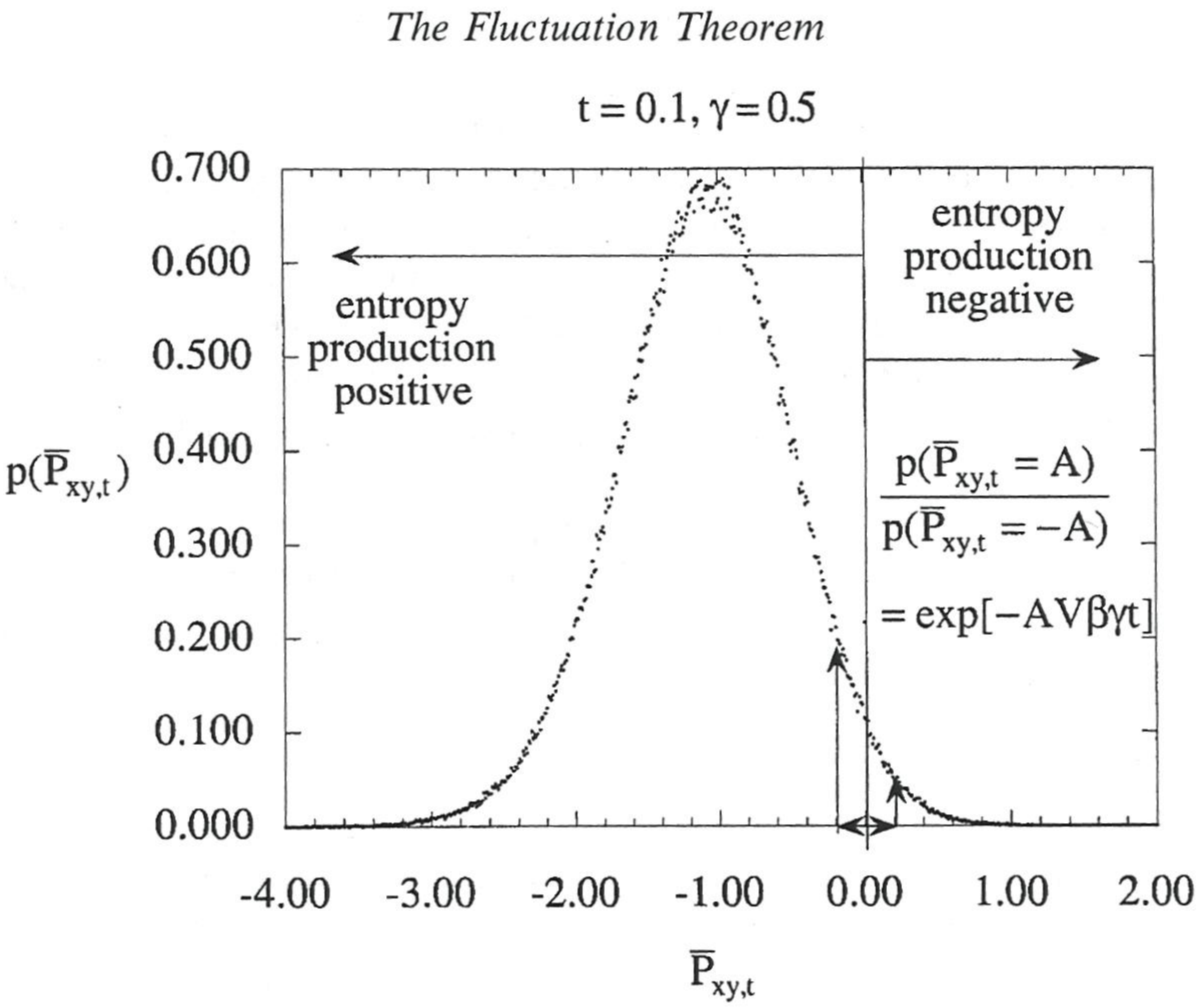
where η is allowed to range from –1.0 to +1.0 in steps of 0.1. For $q = 1.5$ an unweighted fit to $\log\left\langle \varepsilon(r,\eta,t)^q \right\rangle$ versus log r is made, with the slope being $K(q,\eta)$ and the standard deviation being $\sigma(q,\eta)$. A plot of $\log K(q,\eta)$ versus log η yields for our data a collinear region having a positive slope. A weighted linear least squares fit to this region, with weights $K(q,\eta)\ln 10/\sigma(q,\eta)$, has slope α, with the uncertainty represented by the 95% confidence interval returned by the weighted fit.

Eady (1951): ‘I congratulate Dr. Batchelor on his scholarly presentation of the similarity theory of turbulence initiated by Kolmogoroff. The argument which derives the consequences of statistical “de-coupling” between the primary turbulence-producing processes and the secondary small-scale features of the turbulence appears to be sound but does it get us very far? In meteorology and climatology we are concerned principally with the transfer properties of the turbulence, determined mainly by the large-scale primary processes to which the similarity theory does not pretend to apply. It is the great virtue of similarity theories that no knowledge of the mechanism is involved and we do not have to assume anything about the nature of “eddies”; anything which has “size” (such as a Fourier component) will do in our description of the motion. But this emptiness of content is also their weakness and they give us very limited insight. It is true that a similarity theory that could be applied to the *primary* turbulence-producing processes would be of great value but there is no reason to expect that anything simple can be found; when several non-dimensional parameters can be formed, similarity theory, by itself, cannot do much. [continued……]

Similarity theories are attractive to those who follow Sir Geoffrey Taylor in rejecting crude hypotheses regarding "eddies", mixing lengths, *etc.* But those who try to determine the properties of turbulence without such (admittedly unsatisfactory) concepts must show that they have sufficient material (in the shape of equations) to determine the answers. If this is not the case it will be necessary to develop some new principle in addition to the equations of motion and the nature of this principle may be brought to light in a study of the mechanism of the primary turbulence-producing process *i.e.* by trying to refine or modify what we mean by an "eddy" rather than by completely rejecting the concept.'.

A wider context for the importance of understanding the mechanisms of turbulence can be found in Eady and Sawyer (1951).

Evans & Searles (2002), The fluctuation theorem, *Advances in Physics*, **51,** 1529-1585.



The molecular dynamics result that hydrodynamics (organized flow) emerges when a flux causes anisotropy on molecular scales is in contrast to the conventional meteorological decomposition of flow into an organized mean plus dissipative fluctuations (eddies).

On the molecular dynamics view, dissipation is accomplished by the near-average molecules that allow an operational definition of temperature, while the organized flow (wind)is caused by the most energetic molecules producing 'ring currents' with which they are mutually self-sustaining.

Physically, the high speed molecules cause higher number densities ahead and leave lower number densities behind. The random motion of the near-average molecules tends to remove this density gradient, so producing the 'ring current' (vortex in meteorological parlance).

Summary, Lecture 2.1

*** Both microscopic and macroscopic equations have no known analytical solutions: - numerical simulation via computer is necessary.**

•Vorticity emerges from molecular behaviour.

•Non- Gaussian, non-Maxwell-Boltzmann distributions are expected and found in practice.