Preprints (www.preprints.org) | NOT PEER-REVIEWED | Posted: 8 June 2022 doi:10.20944/preprints202206.0128.v1

STRUCTURAL AND DYNAMICAL PROPERTIES OF LIQUID WATER INCREASE TURBULENT FLOWS

Arturo Tozzi
Center for Nonlinear Science, Department of Physics, University of North Texas, Denton, Texas 76203, USA
1155 Union Circle, #311427, Denton, TX 76203-5017 USA
tozziarturo@libero.it

James F. Peters
Department of Electrical and Computer Engineering, University of Manitoba
75A Chancellor's Circle, Winnipeg, MB R3T 5V6, Canada and
james.peters3@umanitoba.ca

Lucio Mariniello
Department of Pediatrics, University Federico II, Naples
lucio.mariniello@unina.it

ABSTRACT

Turbulence is a fluid dynamic problem refractory to mathematical treatment. Examining a theoretical model of liquid water flowing in a cylinder at different Raleigh numbers, we propose a novel approach to elucidate the first stages of turbulent flows. The weakly bonded molecular assemblies of liquid water form a fluctuating branched polymer in which every micro-cluster displays different density. Against the common view of liquid water as an incompressible and continuous fluid, we suggest that the occurrence of transient local aggregates could be able to generate the vortices and eddies that are the hallmarks of turbulence. We quantify the local changes in velocity, diameter and density required to engender "obstacles" to the average flow. Then, we show how these microstructures, equipped with different Raleigh numbers and characterized by high percolation index, could generate boundary layers that contribute to micro-vortices production. We conclude that the genesis of turbulence cannot be assessed in terms of collective phenomena, rather is sustained, among many other factors, by the underrated microscopic inhomogeneities of fluids like liquid water.

KEYWORDS: Reynold number, high-density water, molecular dynamics, water model, percolation theory.

INTRODUCTION

Turbulence is a dissipative phenomenon characterized by mathematically untreatable fluctuating instabilities. Various interacting factors, such as linear dimension, inertial forces, density gradients and mass/heat/momentum random transport provide turbulent flows with intrinsic unpredictability. One of the major difficulties in forecasting turbulent flows is the breakdown of the continuum flow assumption that is a hallmark of the Navier-Stokes equations (Barber and Emerson, 2002). One of the most studied examples of turbulence consists of incompressible fluids with constant density impacting solid surfaces, such as airfoils placed in wind tunnels. The more the flow approaches the cylindrical surface, the slower the velocity. The separation of the fluid's boundary layer from the solid surface leads to unsteady flow conditions and onset of one of the hallmarks of turbulence, i.e., the occurrence of vortices, eddies and swings at different length scales (Sturm et al., 2012). Overflowed surfaces are subject to counter-rotating foci, separation and saddle points, extinction and even inversion of the velocity (Ma et al., 2020) that lead to turbulent flows' production, redistribution and dissipation. Transition from laminar flow to turbulence produces distinct stages of expanding fluctuations regions (Cerbus et al., 2019) where large vortices break up to form smaller ones, locally transferring the kinetic energy in a cascading waterfall devoid of long-range transfers (Kalmár-Nagy and Bak, 2019; Ortiz-Suslow and Wang, 2019).

Here we suggest a novel fluid dynamic approach to quantify the occurrence of micro-vortices in turbulent flows. Concerning the fluid to assess, our choice falls on liquid water, because it consists of a transient dynamical network of fluctuating non-covalent, hydrogen-bonded links (Al-Hamdani and Tkatchenko 2019; Lodish et al., 2000). Contrary to the common approach that regards liquid water as an incompressible, isotropic and homogeneous fluid assessable through continuous models (Nakayama 2017; Gao et al., 2021), we regard liquid water as a compressible fluid. Indeed, water consists of a mixture of low-density water (LDW) and high-density water (HDW) transient assemblies (Muthachikavil et al., 2022) that generate patchy network inhomogeneities and micro-variations in local density which can be assessed just through discretized models. Focusing on a simple model of distilled liquid water flowing in a cylinder, we provide numerical simulations that illustrate how the everchanging, amorphous network configuration of liquid water could

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contribute to generate micro-vortices. In sum, we suggest that that the occurrence of transient networks fluctuating between reversible LDW and HDW assemblies might explain crucial features of turbulent flows in liquid water.

IS LIQUID WATER MADE OF MICRO-ASSEMBLIES?

The first step is to describe and quantify the structural and dynamical properties of liquid water, focusing on the theoretical occurrence of transient micro-assemblies.

Premise: the structural heterogeneity of liquid water. Since hydrogen-bonds are continuously assembled and disassembled, various geometric manifolds have been proposed to describe the water's branched polymer (Shiotari and Sugimoto, 2017). Water polymorphisms have been generally studied in extreme settings (Mariedahl et al., 2019) such as supercritical water (Skarmoutsos and Samios, 2016), high-pressure crystals in supercooled water (Kim et al., 2009; Lin et al., 2018), frozen water confined in nanometric slit pores (Koga et al., 2020), nanochannels formed of cubic crystalline phases **(**Das et al., 2019). Nevertheless, a few studies focused on the micro-structure of liquid water at ambient temperature and pressure. Every water molecule forms a maximum of four hydrogen bonds with the surrounding water molecules, producing a tetrahedral structure (Fanetti et al., 2014; Liu et al. 2017; Milovanović et al., 2020). Thaomola et al. (2017) proposed "short-live" and "long-live" exchange periods with fluctuations in hydrogen bonds' number from 2 to 6, with the nearest neighbors either "loosely" or "tightly" bound to a central water molecule. According to Shiotari and Sugimoto (2017) and Formanek and Martelli (2020), liquid water is composed of assemblies of pentagonal and hexagonal rings, while Liu et al. (2017) pointed towards a dynamical mixture of tetrahedral molecules and ring-and-chain-like structures that produce a densely connected, spherical core of ≈140 water molecules surrounded by a fuzzy zone of ≈1800 loosely connected molecules. According to Naserifar et al. (2019), strong hydrogen bonds at room temperature form multibranched polymers consisting of 151 H_2O molecules per chain, while Ansari et al. (2018) proposed that density fluctuations in liquid water create regions of empty spaces in the shape of spherical or fractal-like voids. In turn, dos Santos et al. (2002) described at ambient conditions the existence of a giant cluster percolating the whole system and Jedlovszky et al. (2007) noticed that tree structure of the largest water cluster is dominated by a linear, chain-like arrangement.
The so called "two-liquids scenario" theorizes the occurrence in water of two competing local molecular structures characterized by low (LDW) and high local density (HDW). Differences in densities, easier to detect in extreme settings, have been described even in liquid water at ambient conditions (Cheng et al. 2019). HDW is regarded as a high-entropy unstructured state, while LDW is believed to display ordered gaps between the first and second molecular shell (de Oca et al., 2019). Camisasca et al. (2019) suggested that HDW could be formed by chains, while LDW by fused dodecahedra working as templates for tetrahedral fluctuations. It is believed that HDW patches tend to be more tetrahedral (Ansari et al., 2018) and to display higher connectivity than LDW patches (Faccio et al., 2022). Cheng et al. (2019) identified also a third type of local structure in liquid water, characterized by ultra-high density and more stable hydrogen bonds.

We regard LDW and HDW assemblies as unnoticed "impurities" in the ever-changing three-dimensional structure of liquid water. These impurities might lead to tiny variations in density that generate micro-surfaces and local modifications of the average macroscopic flow. It is well-known that the addition of impurities induces strong fluctuations in stable and laminar fluid flows and that tiny amounts of long-chain flexible polymers dissolved in turbulent fluids can drastically change flow properties (Zhang et al., 2021). In sum we hypothesize the occurrence in liquid water of tiny micro-assemblies (henceforward MA) able to generate micro-vortices in turbulent flows, characterized by:

a) Density higher or lower than the average density of the whole liquid.
b) Slight variations in fluid velocity compared with the average velocity of the whole liquid.

Experimental setting. Our aim is to evaluate whether microscopic, weak, non-covalent interactions taking spontaneously place in liquid water might produce macroscopic turbulent flows. We are required to build a simulated system to assess and quantify the structural and dynamical properties of microscopic liquid water. We suggest a system consisting of distilled water at temperature = 283.15 K and pressure = 1 Atm, flowing inside a cylinder of diameter L = 1 meter. Water flow is induced by a force constantly exerted at the proximal cylindrical end. The best available quantitative approach to tackle the complexity of turbulent flows consists of the dimensionless Reynolds number (henceforward Re), which describes the ratio of inertial/viscous forces:

$$\mathrm{Re} = \frac{\rho \cdot L \cdot u}{\mu}$$

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where ρ is the fluid density (kg/m^3), L is the characteristic linear dimension (the cylinder's diameter in m), u is the fluid velocity (m/s) and μ is the dynamic viscosity (kg/m · s). Re differentiates between laminar (Re < 2,100) and turbulent flows (Re > 3,000). The cylinder must be smooth and carefully aligned so that turbulent slugs appear naturally at Re > ~3,000 (Wygnanski and Champagne, 2006). Simulations can be performed through freely available calculators, such as, e.g., https://www.omnicalculator.com/physics/reynolds-number. It is well-known that transition to turbulence could be initiated at low Re by introducing modifications in the physical parameters ρ and/or u. In our suggested simulation, the dynamic viscosity ($\bar{\mu}$ = 0.001308 Kg/m s) is held constant, while the average fluid density ($\bar{\rho}$ = 999.7 kg/m^3), the average fluid velocity ($\bar{u}$ = 0.1) and the cylinder diameter L can be modified ad libitum. A few theoretical results are illustrated in **Figure**.

In sum, we suggest that appropriate changes in the parameters L, u, ρ might lead to the formation of MA, i.e., local assemblies of liquid water characterized by physical features that are different compared with the average flow.

Micro-assemblies in liquid water? To assess whether the local features of liquid water could generate MA, a comparison is required between our simulations and the real physical parameters of liquid water. The size of a water molecule is ~2 Å (magnitude: 1 x 10^{-10} meters), while the size of LDW and HDW patches encompasses short (0.3-0.5 nm) as well as long (1-2 nm) assemblies (magnitude: ~1 x10^{-9} meters) (Ansari et al., 2018). Note that the shorter is the MA diameter L, the more laminar is the flow. This means that slight changes in u and ρ in confined zones with low L may cause local modifications in the Reynolds number (**Figure**).

In confined liquid water near ambient temperature and pressure, the average density $\bar{\rho}$ is LDW = 0.78 g/cm^3, while HDW = 1.08 g/cm^3 (Nomura et al., 2017). Therefore, microscopic patches of different density and length can form tiny islands of laminar flows inside turbulent flows.

Even though multiple noncovalent bonds in liquid water at room temperature have an existence briefer than 200 femtoseconds (200 x 10^{-15} seconds) (Lodish et al., 2000; Bakó et al., 2013; Naserifar et al, 2019), LDW has been found to last ~half a second at 160 K (Lin et al., 2018). Therefore, despite their brief existence (Camisasca et al., 2019), HDW and LDW could produce local changes in density that affect upon local environment's dynamics (Skarmoutsos and Samios, 2016) and lead to macroscopic modifications of chemical and biophysical processes (Fanetti et al., 2014). Another factor must be considered when assessing turbulent flows, i.e., the average fluid velocity. Since we do not assume that the flow is constant and uniform, we suggest that every micro-volume could display different velocity.

In sum, transient assemblies do occur in liquid water. The physical micro-structure of liquid water displays magnitude parameters that permit the formation of MA. We will see in the sequel how MA might contribute to modify the mainstream flow, leading to the onset of micro-turbulences.

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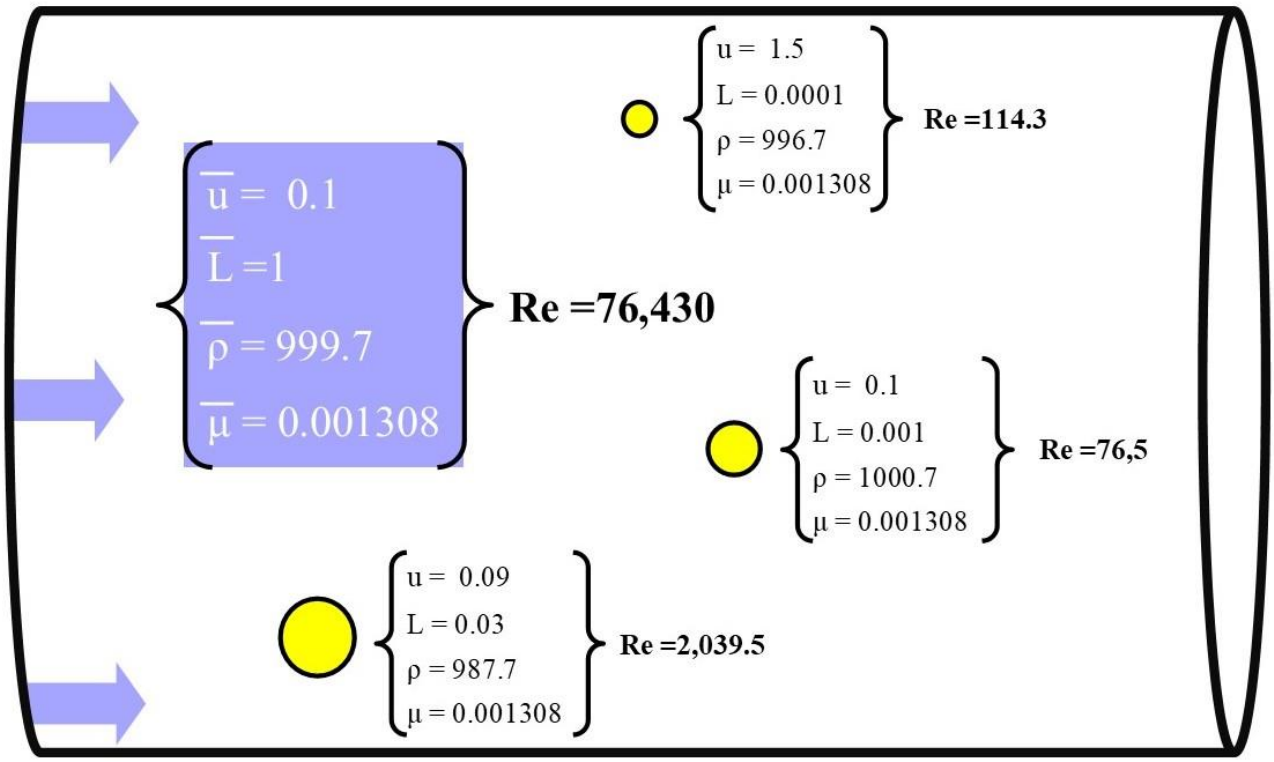

Figure. Schematic illustration of the flow of distilled liquid water at 283.15 K in a cylinder of 1 meter of diameter. The average values of the assessed parameters (blue box) generate a turbulent flow ($\overline{Re}$ = 76,430). The three yellow disks describe transient islands in which micro-assemblies generate flows with different Re numbers.

CAN MICRO-ASSEMBLIES GENERATE MICRO-VORTICES?

Once attained that MA might exist in liquid water, the next step is to assess their potential ability to generate micro-vortices in turbulent flows. We suggest that MA stand for "impurities" that provide micro-obstacles to the main flow and therefore generate vortices. The occurrence of MA's liquid layers gives rise to boundary layers, i.e., liquid water layers in which the fluid velocity is close to zero in the vicinity of MA. Changes in drag between the boundary layer and the undisturbed flow lead to micro-forces acting opposite to the average motion of the fluid. This leads to the production of micro-vortices that can be analytically assessed through the available vorticity equations. When a uniform flow approaches the boundary of a solid body, the fluid particles closest to the body surface describe two simultaneous paths:

a) A path along the x axis, parallel to the body surface.
b) Another path along the y axis, normal to the body surface.

When the flow impacts the object along the x axis in the same direction of the current, vorticity equations describe the fluid's infinitesimal bidimensional surface dx Δy. The subsequent potential flow is characterized by two stagnation points:

a) an anterior stagnation point r.
b) A posterior stagnation point r + Δr, where backflow takes place just downstream from the separation front.

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The vorticity is:

$$\omega = \frac{1}{\Delta r} \frac{d\bar{r}}{dt}$$

Where ω is the total vorticity in a point of the body's profile surface, Δr is the local thickness of the fluid layer close to the body surface and $\bar{r}$ is the curvilinear abscissa along the flow profile.
At low Re, the first slight modifications towards instability take place in the vicinity of the intrerface. Then, turbulent slugs progressively fill the entire cylindrical cross-section as they proceed downstream, growing in length and decreasing in velocity (Wygnanski and Champagne, 2006). Flow evolution is characterized by a phase space trajectory containing many recurrence patterns that convey the interactions among turbulent eddies (Wygnanski and Champagne, 2006). The number of self-crossings in each recurrent loop reflects the temporal complexity: a significant number of simpler trajectories have just a few self-crossings, while a small number of complex trajectories contain > 100 self-crossings (Wu 2020). In touch with our suggestion that MA could generate macroscopic behaviour, it has been demonstrated that local micro-defects in water layers growing on metal surfaces deeply modify the wetting processes (Gao et al., 2021).

Could micro-aggregates modify turbulent flows in liquid water? The occurrence of laminar MA inside turbulent flows is much easier to achieve than the occurrence of turbulent MA inside laminar flows. As stated above, the smaller the dimension L, the more the flow is laminar. Therefore, very small MAs must be islands of laminar flow. If the MA dimension is not far from to the average free path of the fluid molecules, the fluid can no longer be regarded as being in thermodynamic equilibrium. This leads to a non-continuum regime that influences velocity profiles, mass flow rates and boundary shear stresses (Barber and Emerson, 2002). Therefore, when small obstacles such as MAs are introduced into the main flow, turbulences must be observed far downstream.

In order to affect the formation of macroscopic turbulences, short-lived clusters are required to form a wide network able to interact with the average flow. It is known that large connectivity in high-density assemblies leads to percolation inside three-dimensional water lattices (Timonin 2018). Does percolation really occur in water? The answer is positive (Bernabei and Ricci, 2008; Strong et al., 2018). For instance, percolation transition of hydrogen bond networks has been demonstrated in supercritical water, preferentially at high molecular densities (Jedlovszky et al., 2007). Percolation thresholds and cluster size distribution follow a universal power law rule, such that percolation transition occurs when the fractal dimension of the largest cluster reaches the value of 2.53 (Galam and Mauger, 1996; Jedlovszky et al., 2007). Simulations for liquid water suggest that initially disconnected clusters suddenly produce at cut-off values a large space-filling percolating network, in which just a few disconnected fragments/polygonal closures can be found (Geiger 1978). Bearing in mind that 18,01528 grams of water encompass $6{,}02214076\times10^{23}$ water particles, the number of percolating molecules is very high. Indeed, the probability of finding a cluster that spans the three-dimensional system reaches 0.65 in liquid water (Oleinikova et al., 2002). The occurrence of percolation provides an obstacle to the average flow, considering that the bond energies of liquid water assemblies are done in such way as to hinder the main flow and cause turbulence. The energy of a water's hydrogen bond is 1-5 kcal/mol, much lower than the energy of ≈110 kcal/mol required to break a single covalent bond (Lodish et al., 2000). Being the molecular average kinetic energy of ~0.6 kcal/mol at room temperature, many molecules have enough energy to break the noncovalent bonds (Lodish et al., 2000). This means that liquid water flows can be influenced by obstacles made by hydrogen bonds.

In sum, simultaneous variations of different physical parameters generate transient micro-zones of laminar flow inside turbulent flows. When these small obstacles are introduced into the main flow, turbulences can be observed far downstream.

CONCLUSIONS

Turbulence is a widespread phenomenon that can be found in unexpected contexts too, such as, e.g., the intracytoplasmic medium (Fan et al., 2011; Kalmár-Nagy and Bak, 2019; Beppu et al., 2021) and the EEG waves (Sheremet et al., 2019). Occurring more rapidly than molecular diffusion, turbulent flows are crucial for rapid mixing and transport in systems dealing with combustion, pollutant/contaminant reduction, etc. Still, studies concerning turbulent flows are plagued by lack of knowledge of the subtending mathematics. We suggest that the occurrence of turbulent flows can be sustained, among other factors, by the underrated, transient microscopic "impurities" occurring in almost all the fluids. Flows are usually deemed incompressible when the Mach number (the ratio of the flow velocity past a boundary to the local speed of the sound) is smaller than 0.3. Nevertheless, we suggest that the fluid in turbulent systems should be considered, contrary to the common belief, inhomogeneous and compressible. The most of the fluids in which turbulent flows arise

are not isotropic and homogeneous, rather encompass scattered "singularities", "impurities" and "holes" behaving like seeds that contribute to the generation of chaotic flows.
The assembly of large clusters can be methodologically used to discretize continuous liquids. The Knudsen number determines whether statistical mechanics or the continuum mechanics formulation of fluid dynamics should be used to model a system (Barber and Emerson, 2002). The Knudsen number (Kn) is a dimensionless number defined as follows:

$$Kn = \frac{\lambda}{L}$$

Where λ is the average free path i.e., the average distance over which a fluid particle travels before changing its direction/energy as a result of collisions with an obstacle. When the Knudsen number is ≥ 1, the average free path is comparable to the length scale of the problem and the continuum assumption of fluid mechanics is no longer a useful approximation. In such cases, statistical methods should be used.

Among the countless fluids, here we focus of liquid water, which is chemically characterized by intrinsic inhomogeneity. Liquid water could be regarded as a three-dimensional structure where microscopic local changes in density take place. We hypothesize that local micro-defects in the water's polymer might contribute to the making and fuelling of turbulent flows. We suggest that crucial features of turbulence in liquid water, i.e., the vortices, might be explained by the occurrence of transient networks of LDW and HDW assemblies.

This work has some limitations. The phase spaces where water's transient assemblies are believed to occur are difficult to explore, leading to the upsetting concept of "water's no-man's land" (Lin et al., 2018). Despite liquid water can be tackled in terms of a dynamically evolving, fluctuating, branched polymer (Naserifar et al, 2019), a full understanding of its dynamical and structural properties is still lacking (Fanetti et al., 2014) due to technical difficulties in gaining experimental information on ultrafast interplay (Tamtögl et al., 2020). Weak, non-covalent interactions have been studied just in small molecular complexes, falling short of the macroscopic structural properties (Al-Hamdani and Tkatchenko, 2019) that are typical of complex soft materials such as, e.g., supramolecular aggregates. To make things more complicated, totally different networks topologies and physical interpretations have been provided, depending on how rings have been counted (Das et al., 2019; Formanek and Martelli, 2020). The heterogeneity of water is generally approached through simulation of molecular dynamics, such as, e.g., conventional QM/MM scheme and ONIOM-XS methods (Thaomola et al, 2017), second-order Møller–Plesset perturbation theory (Liu et al. 2017), quantum Monte Carlo, non-canonical coupled cluster theory (Al-Hamdani and Tkatchenko, 2019), modified Louvain algorithm of graph community (Gao et al., 2021), topological local (clustering coefficient, path length and degree distribution) and global (spectral analysis) properties (dos Santos et al., 2002; Carreras et al., 2008; Steinberg et al., 2019), persistent homology methods (Wu 2020) and so on.
It is unclear whether the water in the liquid state displays randomness or long-range interactions. For instance, dos Santos et al. (2002) suggested that the water network's behaviour at room temperature is very similar to a Poisson distribution compatible with a random graph. On the contrary, some authors are opposed to purely random arrangements of water assemblies, pointing towards medium- to long-range order (Faccio et al. (2022). To provide a few examples, Tamtögl et al. (2020) suggested that the motion of water at the surface of a topological insulator displays signatures of correlated motion instead of Brownian motion, while Ansari et al. (2018) and Gao et al. (2021) observed collective translational fluctuations of hydrogen-bonded rings and clusters of water molecules. Concerning percolation approaches to liquid water, the limit is that the percolation threshold cannot be accurately located through the cluster size distribution (Jedlovszky et al., 2007). Furthermore, in the assessment of LDW and HDW, the temperature must be taken into account. Since the lower the temperature, the higher the energy linking the hydrogen bonds, increases in temperature upon melting lead to quick drops in the average number of assemblies (Gao et al., 2021) and broader ring size distribution (Bakó et al., 2013; Naserifar et al, 2019). Therefore, microscopic assemblies in water are not easily indistinguishable beyond the isochore end point of 292 K (Nomura et al., 2017).

A world should be spent for the next-to-come developments, in particular topological analysis. A topological approach is mandatory to assess crucial attributes of turbulent systems such as the Laplacian spectra of the network, the average localization distribution of nodes, the local cyclic/bonding coefficients and the vortices features (e.g., the neighbour number and the cycle size distribution) (Bakó et al., 2013). It might be hypothesized that laminar flows stand for symmetry, while turbulent flows stand for symmetry breaks. This means that the interplay between vortex stretching, sourcity and flow symmetry might allow a classification and a mathematical treatment of different kinds of inflow and outflow vortices (Nakayama 2017). To provide an example, flow symmetry of weak vortices is correlated with swirlity development or decay, while stronger vortices lack flow symmetry for inflow in all directions (Nakayama 2017). The last, but not the least, the use of Betti numbers might provide details of the vortical flows' features in turbulent systems. Indeed, Betti numbers can be used to count either the number of water impurities, or the number of micro-vortices generated in turbulent flows.

REFERENCES

1) Al-Hamdani Ys, Tkatchenko A. 2019. Understanding non-covalent interactions in larger molecular complexes from first principles featured. J. Chem. Phys. 150, 010901 (2019); https://doi.org/10.1063/1.5075487.
2) Ansari N, Dandekar R, Caravati S, Sosso GC, Hassanali A. 2018. High and low density patches in simulated liquid water. J Chem Phys. 149(20):204507. doi: 10.1063/1.5053559.
3) Bakó I, Bencsura Á. Hermannson K, Bálint S, Grósz T, et al. 2013. Hydrogen bond network topology in liquid water and methanol: a graph theory approach. Physical Chemistry Chemical Physics. Issue 36, 2013
4) Barber RW, Emerson DR. 2002. The Influence Of Knudsen Number On The Hydrodynamic Development Length Within Parallel Plate Micro-channels. WIT Transactions on Engineering Sciences. Volume 36, DOI10.2495/AFM020191
5) Beppu K, Izri Z, Sato T, Yamanishi Y, Sumino Y, Maeda YT. 2021. Edge current and pairing order transition in chiral bacterial vortices. Biophysics And Computational Biology. 118 (39) e2107461118. https://doi.org/10.1073/pnas.2107461118.
6) Bernabei M, Ricci MA. 2008. Percolation and clustering in supercritical aqueous fluids. J. Phys.: Condens. Matter 20 494208.
7) Camisasca G, Schlesinger D, Zhovtobriukh I, Pitsevich G, Pettersson LGM. 2019. A proposal for the structure of high- and low-density fluctuations in liquid water. J. Chem. Phys. 151, 034508; https://doi.org/10.1063/1.5100875.
8) Carreras BA, Llerena I, Garcia L, Calvo I. 2008. Topological characterization of flow structures in resistive pressure-gradient-driven turbulence. Phys. Rev. E 78, 066402
9) Cerbus RT, Sakakibara J, Gioia G, Chakraborty P. 2019. The turbulent flow in a slug: a re-examination. Journal of Fluid Mechanics. Volume 883.
10) Das K, Roy B, Satpathi S, Hazra P. 2019. Impact of Topology on the Characteristics of Water inside Cubic Lyotropic Liquid Crystalline Systems. J. Phys. Chem. B 2019, 123, 18, 4118–4128. https://doi.org/10.1021/acs.jpcb.9b01559.
11) de Oca JMM, Accordino SR, Verde AR, Alarcón LM, Appignanesi GA. 2019. Structural features of high-local-density water molecules: Insights from structure indicators based on the translational order between the first two molecular shells. Phys. Rev. E 99, 062601.
12) dos Santos VML, Moreira FGB, Longo RL. 2004. Topology of the hydrogen bond networks in liquid water at room and supercritical conditions: a small-world structure. Chemical Physics Letters, Vol.390, No.1-3, 157-161. DOI10.1016/j.cplett.2004.04.016.
13) Faccio C, Benzi M, Zanetti-Polzi L, Daidone I. 2022. Low- and high-density forms of liquid water revealed by a new medium-range order descriptor. Journal of Molecular Liquids. Volume 355, 118922. https://doi.org/10.1016/j.molliq.2022.118922.
14) Fan X, Ma J, Wan W, Zhang P, Wang C, Wu L. 2011. Increased intracellular calcium concentration causes electrical turbulence in guinea pig ventricular myocytes. Sci China Life Sci. 54(3):240-7. doi: 10.1007/s11427-011-4146-1.
15) Fanetti S, Lapini A, Pagliai M, Citroni M, Di Donato M, et al. 2014. Structure and Dynamics of Low-Density and High-Density Liquid Water at High Pressure. J. Phys. Chem. Lett. 5, 1, 235–240. https://doi.org/10.1021/jz402302z
16) Formanek M, Martelli F. 2020. Probing the network topology in network-forming materials: The case of water. AIP Advances 10, 055205. doi: 10.1063/5.0005332.
17) Gao, Y., Fang, H. & Ni, K. 2021. A hierarchical clustering method of hydrogen bond networks in liquid water undergoing shear flow. Sci Rep 11, 9542 (2021). https://doi.org/10.1038/s41598-021-88810-7.
18) Galam S, Mauger A. 1996. Universal formulas for percolation thresholds. Phys. Rev. E 53, 2177.
19) Geiger A. 1979. Aspects of the percolation process for hydrogen-bond networks in water. J. Chem. Phys. 70, 4185. https://doi.org/10.1063/1.438042.
20) Jedlovszky P, Brovchenko I, Oleinikova A. 2007. Percolation Transition in Supercritical Water: A Monte Carlo Simulation Study. J. Phys. Chem. B 2007, 111, 26, 7603–7609
21) Kalmár-Nagy, T., Bak, B.D. 2019. An intriguing analogy of Kolmogorov's scaling law in a hierarchical mass–spring–damper model. Nonlinear Dyn 95, 3193–3203 (2019). https://doi.org/10.1007/s11071-018-04749-x.
22) Kim CU, Barstow B, Tate MW, Grunera SM. 2009. Evidence for liquid water during the high-density to low-density amorphous ice transition. Proc Natl Acad Sci U S A. 2009 Mar 24; 106(12): 4596–4600. doi: 10.1073/pnas.0812481106.
23) Koga, K., Tanaka, H. & Zeng, X. 2000. First-order transition in confined water between high-density liquid and low-density amorphous phases. Nature 408, 564–567 (2000). https://doi.org/10.1038/35046035.
24) Lin C, Smith JS, Sinogeikin SV, Shen G. 2018. Experimental evidence of low-density liquid water upon rapid decompression. PNAS. 115 (9) 2010-2015. https://doi.org/10.1073/pnas.1716310115.

25) Liu J, He X, Zhang JZH. 2017. Structure of liquid water – a dynamical mixture of tetrahedral and 'ring-and-chain' like structures. Phys. Chem. Chem. Phys. 19, 11931-11936. https://doi.org/10.1039/C7CP00667E.
26) Lodish H, Berk A, Zipursky SL, et al. 2000. Molecular Cell Biology. 4th edition. New York: W. H. Freeman; 2000.
27) Ma A, Gibeau B, Ghaemi S. 2020. Time-resolved topology of turbulent boundary layer separation over the trailing edge of an airfoil. Journal of Fluid Mechanics, Volume 891, A1. DOI: https://doi.org/10.1017/jfm.2020.106.
28) Mariedahl D, Perakis F, Späh A, Pathak H, Kim KH et al. 2019. X-ray studies of the transformation from high- to low-density amorphous water. Philos Transact Royal Society A. Volume 377, issue 2146. https://doi.org/10.1098/rsta.2018.0164.
29) Milovanović MR, Živković JM, Ninković DB, Stanković IM, Zarić SD. 2020. How flexible is the water molecule structure? Analysis of crystal structures and the potential energy surface. Phys. Chem. Chem. Phys., 2020,22, 4138-4143. https://doi.org/10.1039/C9CP07042G.
30) Muthachikavil AV, Kontogeorgis GM, Liang X, Lei Q, Peng B. 2022. Structural characteristics of low-density environments in liquid water. Phys. Rev. E 105, 034604.
31) Nakayama K. 2017. Topological features and properties associated with development/decay of vortices in isotropic homogeneous turbulence. Phys. Rev. Fluids 2, 014701.
32) Naserifar S, Goddard III WA. 2019. Liquid water is a dynamic polydisperse branched polymer. PNAS. 116 (6) 1998-2003. https://doi.org/10.1073/pnas.1817383116
33) Nomura K, Kaneko T, Bai J et al. 2017. Evidence of low-density and high-density liquid phases and isochore end point for water confined to carbon nanotube. PNAS. 114 (16) 4066-4071. https://doi.org/10.1073/pnas.1701609114.
34) Oleinikova A, Brovchenko IV, Geiger A, Guillot B. 2002. Percolation of water in aqueous solution and liquid-liquid immiscibility. The Journal of Chemical Physics 117(7):3296-3304. DOI: 10.1063/1.1493183.
35) Ortiz-Suslow DG, Wang Q. 2019. An Evaluation of Kolmogorov's −5/3 Power Law Observed Within the Turbulent Airflow Above the Ocean. Geophysical Research letters. https://doi.org/10.1029/2019GL085083.
36) Pusztai L. 2000. Comparison between the structures of liquid water and (high- and low-density) amorphous ice. Physical Chemistry Chemical Physics. Issue 12.
37) Sheremet A, Qin Y, Kennedy JP, Zhou Y, Maurer AP. 2019. Are EEG flows turbulent? Front Syst Neurosci. 2018; 12: 62. doi: 10.3389/fnsys.2018.00062.
38) Shiotari A, Sugimoto Y. 2017. Ultrahigh-resolution imaging of water networks by atomic force microscopy. *Nat Commun* 8, 14313 (2017). https://doi.org/10.1038/ncomms14313ù
39) Skarmoutsos I, Samios J. 2016. Local Density Inhomogeneities and Dynamics in Supercritical Water: A Molecular Dynamics Simulation Approach. J. Phys. Chem. B 2006, 110, 43, 21931–21937. https://doi.org/10.1021/jp060955p.
40) Steinberg L, Russo J, Frey J. 2019. A new topological descriptor for water network structure. J Cheminform 11, 48 (2019). https://doi.org/10.1186/s13321-019-0369-0.
41) Strong SE, Shi L, Skinner JL. 2018. Percolation in supercritical water: Do the Widom and percolation lines coincide? J. Chem. Phys. 149, 084504 (2018); https://doi.org/10.1063/1.5042556.
42) Sturm H, Dumstorff G, Busche P, Westermann D, Lang W. 2012. Boundary Layer Separation and Reattachment Detection on Airfoils by Thermal Flow Sensors. Sensors (Basel, Switzerland). DOI:10.3390/s121114292.
43) Tamtögl A., Sacchi M., Avidor N, Calvo-Almazán I, Townsend PSM, et al. 2020. Nanoscopic diffusion of water on a topological insulator. Nat Commun 11, 278. https://doi.org/10.1038/s41467-019-14064-7
44) Thaomola S. Tongraar A, Kerdcharoen T. 2012. Insights into the structure and dynamics of liquid water: A comparative study of conventional QM/MM and ONIOM-XS MD simulations. Journal of Molecular Liquids. Volume 174, October 2012, Pages 26-33.
45) Timonin PN. 2018. Statistical mechanics of high-density bond percolation. Phys. Rev. E 97, 052119.
46) Wu, H. 2020. The topological features of a fully developed turbulent wake flow. APS Division of Fluid Dynamics (Fall) 2020, abstract id.S09.007.
47) Wygnanski IJ, Champagne FH. 2006. On transition in a pipe. Part 1. The origin of puffs and slugs and the flow in a turbulent slug. Journal of Fluid Mechanics. Volume 59, Issue 2. On transition in a pipe. Part 1. The origin of puffs.
48) Yang C, Zhang C, Ye F, Zhou X. 2019. Ultra-high-density local structure in liquid water. Chinese Physics B. 28(11): 116104.
49) Zhang Y-B, Bodenschatzhait E, Xu A.Xi H-D. 2021. Experimental observation of the elastic range scaling in turbulent flow with polymer additives. Science Advances. Vol. 7, No. 14. DOI: 10.1126/sciadv.abd3525.