Detecting structural complexity: from visiometrics to genomics and brain research

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Abstract. From visual inspection of complex phenomena to modern visiometrics, the quest for relating aspects of structural and morphological complexity to hidden physical and biological laws has accompanied progress in science ever since its origin. By using concepts and methods borrowed from differential and integral geometry, geometric and algebraic topology, and information from dynamical system analysis, there is now an unprecedented chance to develop new powerful diagnostic tools to detect and analyze complexity from both observational and computational data, relating this complexity to fundamental properties of the system. In this paper we briefly review some of the most recent developments and results in the field. We give some examples, taken from studies on vortex entanglement, topological complexity of magnetic fields, DNA knots, by concluding with some comments on morphological analysis of structures present as far afield as in cosmology and brain research.

1 Complex structures in nature

This paper presents a rather brief overview of the progress made so far in what we may call *structural complexity analysis* of physical and biological systems. As we shall see, this relies on the mathematical study of aspects associated with such systems, that are eminently morphological in character, by establishing possible relationships between these aspects and fundamental physical properties of such systems. In this sense, structural complexity analysis aims at relating fundamental physical aspects of a complex system with key mathematical descriptors of the morphological complexity that the system exhibits.

At all scales nature shows some degree of organization. On a macro-scale, from the cosmic distribution of mass and energy observed in the filamentary structures present in our Universe [15], to the complex network of plasma loops flaring up in the solar corona [6]. On a human scale, self-organized

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structures are present on a very wide spectrum, fluid flows being perhaps the best prototypes [34]: from snow crystals to cloud formation, from froth and bubbles to eddies, vortices and tornados, sheets of flames, vapor jets, and so on. Similarly on a much smaller scale: polymers in chemical physics [13], human DNA, highly packed in a tiny cell volume [7], or the intricate neuronal network, that wires up our nerve system [14]. Self-organization and co-operative behavior are indeed what ultimately make us living organisms! Self-organization of structures, constituted by mass concentration, plasma particles, fluid molecules, grains, crystals, chemical compounds or living cells, seems indeed to share generic features, inherently associated with their own very existence [4, 24].

Structural organization is just one way to identify such a universal property, and whatever hidden mechanism is in place to produce it, uncovering possible relations between generic properties of structural complexity and physical information is clearly of great importance [19]. Progress in this direction gives us new ways to correlate localization and occurrence of apparently distinct physical and mathematical properties, that may reveal an unexpected new order of things, perhaps at a more fundamental level. Indeed, progress in understanding and detecting levels of complexity of the actual physical system might bring in a new paradigmatic order in the complexity of the mathematical structures that are behind it; and this, in turn, might mean new ways of interpreting relationships between mathematical structures on one hand, and the physical world, on the other.

Before embarking on more specific questions, it is perhaps convenient to explain the general strategy. Let us start with some common definitions of physical "structures": in general these will be defined by some space-time localization and coherency of the constituent physical property, be it a scalar, vector or tensor field. Mass, temperature, magnetic field, vorticity, molecular

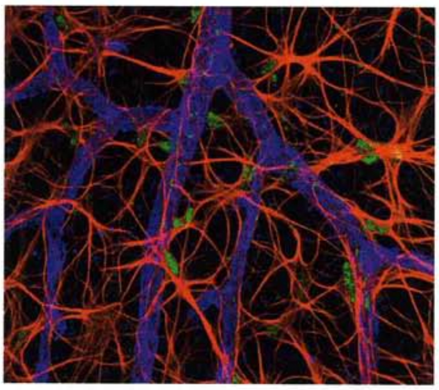

Fig. 1. Structural complexity is naturally displayed in this digital image of a three-dimensional network of retina astrocytes (courtesy of H. Mansour and T. Chan-Ling, Retinal Biology Laboratory, U. Sydney; *Bioscapes* 1st Prize, 2005)

groups, electric currents are, for instance, all possible candidates. What really should matter here is:

- to attain high localization in space; and
- to preserve this localization on some time-scale.

Filaments, flux tubes, hexagonal patterns, sheets or spherical volumes provide the geometric support for some of the examples given above. The state of organization and the degree of order present in a network of such physical structures defines then structural complexity ([26]; see Fig. 1). Our strategy will be to develop and use concepts borrowed from the realm of mathematical sciences, to study fundamental aspects of structural complexity and to draw relationships between this complexity and the physical properties of the system. To do this we need to identify and develop useful mathematical tools. By focussing on aspects of morphological complexity, we intend to leave aside statistical methods, based on information theory and spatial statistics [23], to concentrate on geometric, topological and algebraic information.

In the sections below we shall outline some of the progress made in recent years, rooted in the old-fashioned visual inspection of complex phenomena (§2), to land on current visiometric works (§3). We shall then appeal to some of the current developments in geometric and topological methods (§4) to present new results on applications to vortex dynamics, magnetic fields, DNA genomics and cosmology (§5). An outlook on future developments is presented in §6, speculating on possible applications to ecological and social networks as well as aspects of brain research. Conclusions are finally drawn in §7.

2 A visual approach to structural complexity

From its very origin science has relied on direct visual inspection of complex phenomena. From ancient natural philosophers to modern experimentalists, our eyes and brain are powerful tools of investigation that have forged the progress of science ever since; eyes and memory providing a record, and our brain an amazingly efficient powerhouse for synthesis and elaboration of information. The meticulously accurate drawings of Leonardo da Vinci are notoriously a masterpiece of both artistic geniality and scientific rigorous investigation of nature. His famous *Water Studies* [12], for instance, exemplify our (his!) quest for unveiling the mysteries of nature, through detailed sketching of complex flow patterns: these, being indeed visual aids of investigation, were "visual renderings" *ante litteram.*

This approach continued uninterrupted up to the modern days, til contemporary digital imaging or computational visualization from either observational data (as in cosmology, biology and ethology) or direct numerical simulations of governing equations (as in engineering, meteorology and oceanography). Huge data sets (obtained from satellite missions or genetics laboratories) are being accumulated at an ever faster rate. There is however a lack

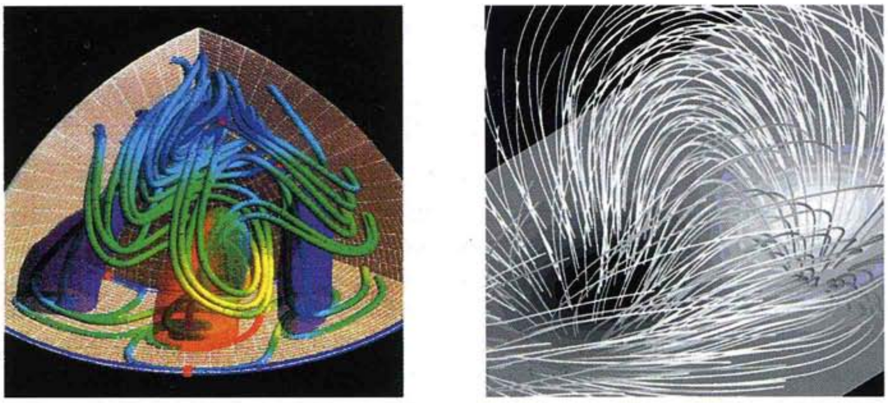

Fig. 2. Examples of visual rendering of (left) enhanced streamlines associated with vortex rolls in a sextant of volume (adapted from Kitauchi et al., RIMS, U. Kyoto & Natnl. Inst. Fusion Sci., Nagoya; *Phys. Today* cover, **12**, 1996), and (right) magnetic fields originating from simulated active regions of sun spots (adapted from Abbett et al., Space Science Laboratory, U. California at Berkeley, 2008)

of diagnostic tools for such a wealth of information. In research areas more closely related to the mathematical sciences, such as magnetohydrodynamics, aerodynamics and plasma physics, elaborate diagnostic toolkits for the analysis of complex fluid flow visualizations (see Fig. 2) have been developed.

3 From visiometrics to complexity analysis

Advanced visiometrics [35] rely indeed on mathematical measures of structural complexity that are at the heart of this novel approach. By exploiting progress made on vector and tensor field analysis of structural classification and stability of dynamical systems [1, 18], flow visualizations can now render three-dimensional complex patterns by various techniques, such as fiber or field-line (stream-, path- or time-line) tracing, arrow plotting, iso-surface and volume rendering. By identifying location and type of critical points, where field lines converge or diverge (such as nodes, foci, centers, saddles, etc.), a feature-based image tensor field is obtained, whose geometric and topological properties are then fully analyzed [17].

From tensor analysis we extract information on eigenvalues and eigenvectors, that can be used to determine anisotropy indices [9, 36] to quantify the degree of isotropy present in the simulation of a physical process (a turbulent flow, a pathogen diffusion, etc.). Eigenvalue analysis is used to distinguish filament-dominated regions from regions where sheets are present. All this is of course a by-product of numerical integration of the governing equations. But in many cases raw data are simply provided by direct recording of natural or experimental observations. Once the data are visualized, we are in

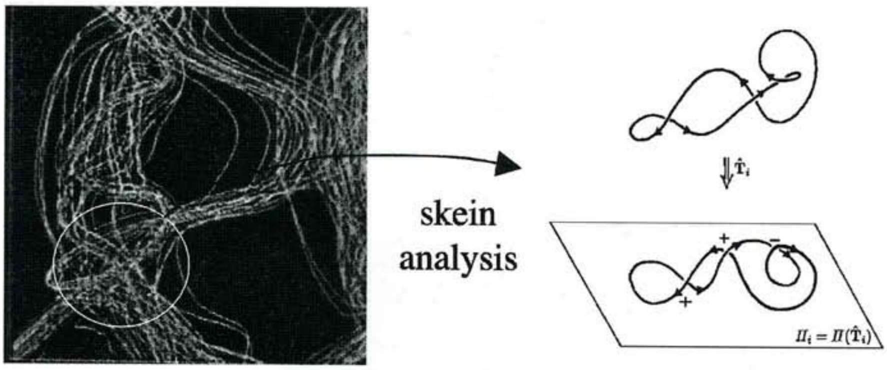

Fig. 3. From direct numerical simulations, a sub-domain is extracted and analyzed by methods of structural complexity analysis

a situation similar to that of Leonardo's *Water Studies*: it is more specifically in this context that morphological measures of structural complexity analysis are fully exploited ([21, 25]; see Fig. 3). A theoretical framework based on concepts borrowed from differential and integral geometry, and algebraic and geometric topology is usefully applied and possibly complemented by information from dynamical systems analysis, i) to describe and classify complex morphologies; ii) to study possible relationships between complexity and physical properties; and also iii) to understand and predict energy localization and transfer. Possible applications include the development of new diagnostic and visiometric tools and the implementation of real-time analysis of dynamical and biological processes.

4 Geometric, topological and algebraic measures

Geometric information is used to quantify shape. For space curves, for example, length, curvature, torsion, writhing and inflexional states, are all important information. Likewise, the integral measures of surfaces and volumes, together with mean and Gaussian curvature. Information obtained from projected diagrams of the original geometric objects can also be useful; in the case of curves we obtain planar graphs made by contour lines (edges) joined at nodal points (vertices) (see diagram on the left of Fig. 3). Depending on the number of arcs incident at the nodal point, we define a degree of multiplicity that can be implemented in a "shaking algorithm" to simplify graph complexity and analysis. Rotation indices are used to weight and sign the area of the sub-regions (faces) of the graph [27, 29]. Shapefinders [30] are used to determine characteristic shapes, going from thin filaments and tubes to sheets and pancakes (see §5.4 and Fig. 9 below).

Topological information is used to qualify shape. The knot theory provides information on knot and link complexity by measures of minimum crossing number, genus, bridge number, knot polynomial, braid index [33]. Other information, coming from linking number, unknotting number, number of prime factors, etc., are useful to complement the description of physical phenomena (linking number information providing a measure for fluid helicity, unknotting number for recombination processes, etc.). For surfaces, orientability,

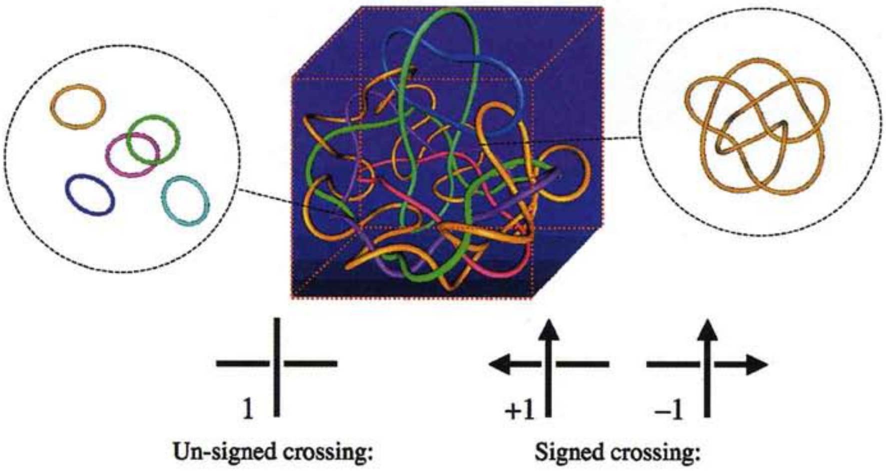

Fig. 4. Information on unsigned and signed crossing numbers can be used to quantify morphological complexity and geometric aspects, such as writhing of filaments

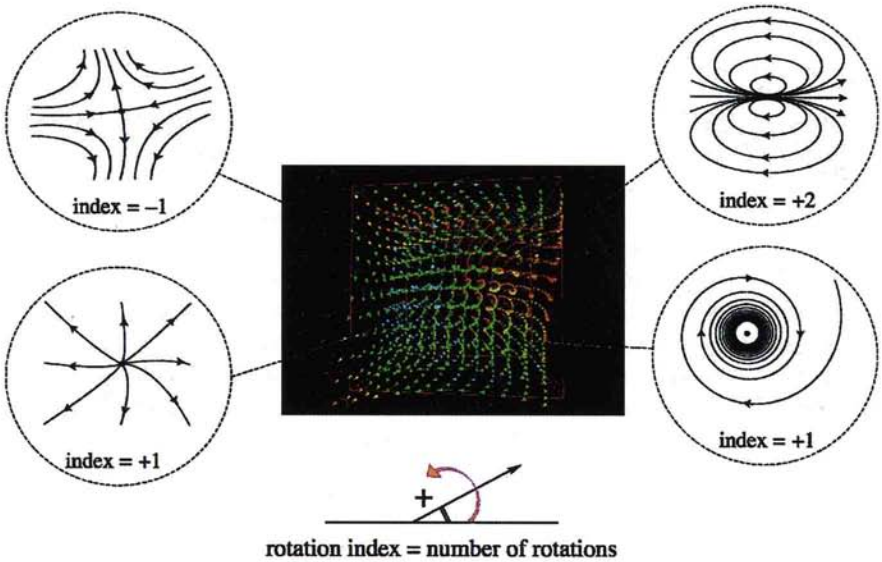

Fig. 5. Algebraic information from dynamical system analysis is provided, for example, by rotation indices associated with vector or tensor field analysis

genus, Betti number and Euler characteristic are all important properties that, as we shall mention in §5.4, help to determine form factors.

The total number of apparent intersections between filament strands in space, averaged over all directions, provides an algebraic measure of complexity and is a good detector of structural complexity [5]. If orientation is physically inherited, then the axial curves identified by the filaments are oriented too and, according to standard convention, an algebraic sign is assigned to each apparent intersection (see Fig. 4). We can then repeat the algebraic counting of the total number of apparent *signed* intersections, and we have an algebraic interpretation of total writhing. If, in place of physical filament tangles, we refer to abstract gaze patterns in visual science [16], we can then relate the complexity of human eye movements to visual perception and information. Finally, in the case of dynamical systems, rotation indices (see Fig. 5) are readily available from vector or tensor field analysis, and these help to classify sub-domains of flow patterns by topology-based methods [17].

5 Examples of applications in mathematical physics, biology, cosmology

Structural complexity analysis finds useful applications in many fields of current research. Here we briefly report on some recent results and current developments in particular areas of mathematical physics, biology and cosmology, to account for some of the progress made so far.

5.1 Energy-complexity relations for vortex tangles

Structural complexity analysis is applied to investigate relationships between dynamical and energy aspects of fluid flows and complexity measures. Numerical tests [5] based on the production of vortex entanglement due to the action of a background super-posed helical flow on seed vortex rings (see Fig. 6), show that a power-law correspondence between complexity, measured by the average crossing number $\overline{C}$, and the kinetic energy E of the system holds true independently from the originating turbulent state. For a tangle $\mathcal{T}$ of vortex lines χ_i ($i = 1, 2, \ldots$), the average crossing number is obtained by computing the sum of all apparent crossings at sites ϵ_r, made by pairs of vortex lines, averaged over all directions, by extending the counting to the whole tangle; this is defined by

$$\overline{C} = \sum_{\{\chi_i,\chi_j\}\in\mathcal{T}} \langle \sum_{r\in\chi_i\#\chi_j} \epsilon_r \rangle \ , \tag{1}$$

where $\#$ denotes disjoint union of all apparent intersections of curve strands, including self-crossings. Kinetic energy, on the other hand, is given by

$$E = \frac{1}{2}\int_{V(\mathcal{T})} \|\mathbf{u}\|^2 \,\mathrm{dV} \ , \tag{2}$$

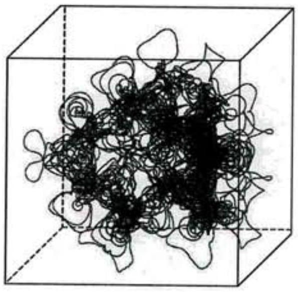

Fig. 6. Vortex tangle produced by interaction and evolution of a superfluid background flow (adapted from [5])

where $V(\mathcal{T})$ is the total volume of the vortex tangle, and $\mathbf{u}$ is fluid velocity. During evolution, entanglement grows and these two quantities change in time t, according to the following relation

$$\overline{C}(t) \propto [E(t)]^2 \ . \tag{3}$$

This result has been confirmed by several tests under different initial conditions and for different evolutions.

5.2 Topological bounds on magnetic energy of complex fields

There has been considerable progress towards foundational issues in topological field theory, including aspects of topological complexity. In the early '90s works by Berger, Freedman & He, Moffatt (see the collection of papers edited by Ricca, [25]) showed that in ideal magnetohydrodynamics the magnetic energy M of a knotted flux tube $\mathcal{K}$, of constant flux Φ and volume $V = V(\mathcal{K})$, is bounded from below by knot complexity. In particular, if magnetic energy is given by

$$M = \int_{V(\mathcal{K})} \|\mathbf{B}\|^2 \,\mathrm{dV} \ , \tag{4}$$

then we have

$$M_{\min} \geq f(\Phi, V)\, c_{\min} \ , \tag{5}$$

where $f(\cdot)$ denotes a given functional relationship, and $c_{\min}$ is the topological (i.e., minimum) number of crossings of knot type $\mathcal{K}$. Another important quantity, related to linking, is the magnetic helicity H, given by

$$H = \int_{V(\mathcal{K})} \mathbf{A} \cdot \mathbf{B} \,\mathrm{dV} \ , \tag{6}$$

where $\mathbf{B} = \nabla \times \mathbf{A}$ (with $\nabla \cdot \mathbf{A} = 0$). For zero-framed knots, by relying on previous results by Arnold, Freedman & He and Moffatt, Ricca [28] has proved that the following inequalities hold true:

$$M \geq \left(\frac{16}{\pi V}\right)^{1/3} |H| , \qquad M_{\min} \geq \left(\frac{16}{\pi V}\right)^{1/3} \Phi^2 \, c_{\min} . \tag{7}$$

Moreover, in the presence of dissipation, magnetic fields reconnect and topological complexity is bound to change according to the following inequality

$$H(t) \leq 2\Phi^2 \overline{C}(t) \tag{8}$$

hence providing an upper bound to the amount of magnetic helicity and average linking of the magnetic system.

5.3 DNA knots and links

In recent years there has been growing confidence that at various levels of investigation morphological and structural properties of DNA conformation are not only visibly present and physically relevant, but also key to influence biological functions as well [10]. In this direction a great deal of work is carried out on DNA knots and links, in relation to fundamental biological aspects, including enzymatic action, protein coding and packing [33]. Fig. 7, for example, shows the relative distribution of specific DNA knot types extracted from the phage capsid of bacteriophage P4. This kind of research is a typical example of combination of experimental laboratory work and data analysis based on pure topological information.

The topological complexity of DNA catenanes, on the other hand, changes by the enzymatic actions performed by the topoisomerase. Here, local pro-

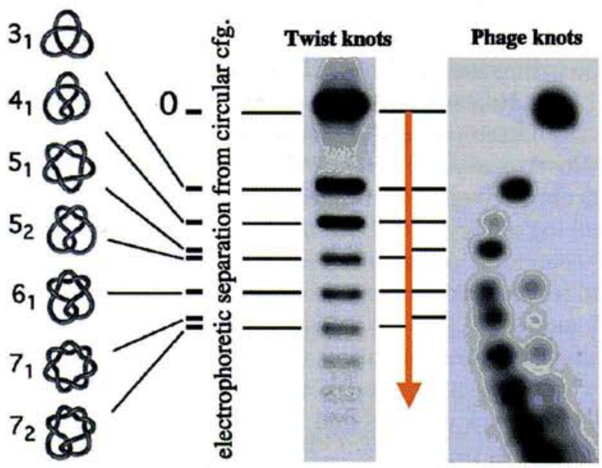

Fig. 7. Identification of DNA knot types by electrophoretic separation during migration in the gel (adapted from [3])

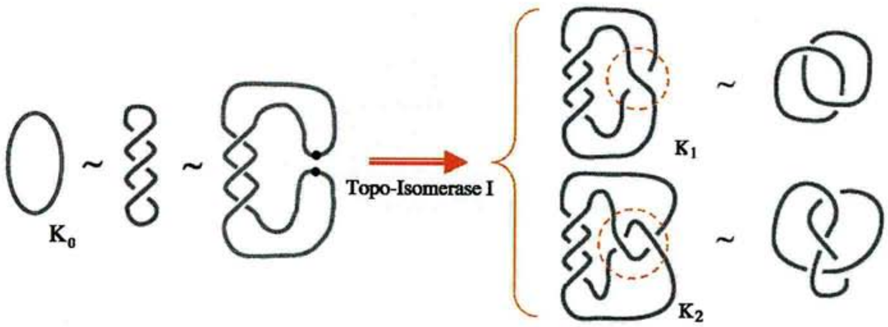

Fig. 8. After performing twist moves on the unknot (K_0), a reconnection on a local site gives the Hopf link K_1; after a second twist move, followed by another reconnection, we obtain the four-crossing knot K_2 (adapted from [20])

cesses of "cut-and-connect", performed locally by these actions on DNA strands to do, or to undo, DNA knots and links, may be modeled by applying the tangle theory (see Fig. 8, and the recent review by [20]). An interesting implementation of this technique [11] has led, for instance, to the development of dedicated software (such as Bob Scharein's KnotPlot) for computational simulations.

5.4 Complexity analysis of cosmological data

One of the most challenging problems in cosmology is the formation and distribution of the large-scale structure of the Universe. In recent years the problem of analyzing the wealth of information based on observational data of galaxy distribution has received new impetus, thanks to the application of morphological detectors (Minkowski functionals), coming from integral geometry [22]. In low dimensions, these actually reduce to the standard measures of volume V, bounding surface A, global mean curvature H and Euler characteristic χ, the latter providing eminently topological information on the distribution set. A combined used of these measures has become a powerful tool to detect morphological complexity associated with a point distribution set. By identifying galaxy distribution with the corresponding distribution of the galaxies' centers of mass, these measures find application to determine geometric and topological properties of cosmic clusters (for example, by using "germ-grain" models).

A morphological characterization of structures is obtained by the use of "shapefinders", to detect degrees of filamentarity F and planarity P, from spheroidal distributions of mass and energy. By defining length, width and thickness respectively by

$$L = \frac{H}{4\pi\chi} , \qquad W = \frac{A}{H} , \qquad T = \frac{3V}{A} , \tag{9}$$

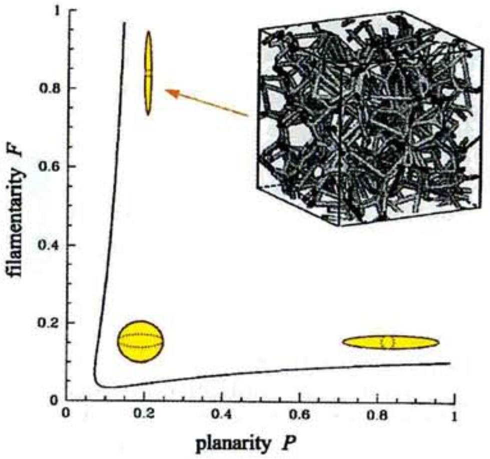

Fig. 9. Blaschke diagram applied to morphological analysis of disordered medium. Inset illustrates a case of computational simulation of structural growth of Voronoi model with 100 seeds on a 200^3 lattice (adapted from [2])

we have [30]

$$F = \frac{L - W}{L + W}\,, \qquad P = \frac{W - T}{W + T}\,, \tag{10}$$

used to determine the morphological characteristics in a wide range of applications: structures that are predominantly filament-like being characterized by $F \approx 1$ and $P \ll 1$, and sheet-like structures being characterized by $P \approx 1$ and $F \ll 1$. In general, for convex bodies we have $P \geq 0$ and $F \leq 1$ (for a sphere $P = F = 0$), with plots of F versus P denoting Blaschke diagrams of form factors. An example is shown in Fig. 9, where dominant morphological characteristics are evidenced by the curve in the (F, P) plane. As we see, by changing parameters one can go from high filamentarity (tube-like shapes) to high planarity (sheet-like shapes or pancakes), passing through spheroidal shapes (bulkiness). These measures can be related to morphological detectors associated with dynamical systems either based on data extracted from field line tracing [29] or, for example, based on eigenvalue analysis of corresponding fluid flows [35].

6 Outlook: morphological complexity for brain research

With increasing storage capability and computational power there will be an ever greater demand for effective diagnostic tools to analyze and detect properties of structural complexity in relation to physical and biological properties. Applications of complexity measures like average crossing number and shapefinders find already new applications in the morphological analysis of

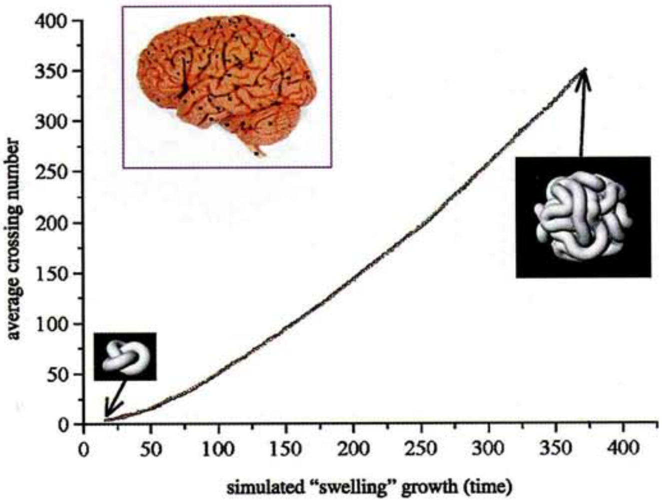

Fig. 10. Simulation of "swelling" growth of a complex surface: the initial, relatively simple morphology (here simply measured by the average crossing number) increases with the simulated inflationary process of growing complexity (collaborative work in progress; adapted from P. Pieranski, Laboratory of Computational Physics and Semiconductors, Poznan University of Technology, 2007)

such disparate areas as the study of disordered media (including particle-based structures, amorphous micro-structures, cellular and foam-like structures; see, for example, [2] and Fig. 9 above), isotropic turbulence or magnetic field generation [37]. Work is in progress on possible future applications of these methodologies to the new frontier of neural networks and brain research. For instance, work done in collaboration with this author may include analysis of possible relationships between structural complexity measures and generic features associated with the growth of a bounding surface to model early stages of brain development (see Fig. 10). Other possible applications may well include studies of generic features common to nerve and blood vessel wiring in the human body [8], complex networking in the world-wide-web, the predator-prey chain system or the social system, that, contrary to intuition, seem to show a remarkable common degree of self-organized dynamics on all length scales [32].

7 Conclusions

In this paper we have shown how work on structural complexity, and in particular analysis on morphological aspects based on geometric, topological and algebraic information, may offer powerful tools to investigate relationships between complexity features and energy localization or functional activity.

Examples of recent applications include vortex tangle analysis in fluid dynamics, energy bounds for magnetic braids in solar physics, DNA knots and links in ultrastructural biology, morphological complexity analysis in astrophysics, cosmology and disordered media. In the future, likely applications will include the study of the development of neural systems, brain formation, and complex networks such as the world-wide-web.

These studies will certainly benefit from novel diagnostic tools based on structural complexity analysis and possibly new morphological detectors. This approach alone, however, cannot be sufficient, if not supplemented by fundamental work on constitutive laws and governing equations. Hence, if structural complexity analysis may represent a preliminary and necessary step towards a more comprehensive understanding of complex phenomena, it is actually in disclosing the relationships between morphological aspects and functional issues that this approach proves most useful. It is in this direction that old and new mathematical concepts will find their best use.

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