Chapter 8

Conclusions and Future Work

8.1 Geometry of individual structures

A methodology for the identification of structures based on their geometry has been introduced first. Our goal has been to develop a methodology that can compensate for the computational bottleneck of DNS computing for turbulent flows, and to provide a solid mathematical framework for non-local characterization of the flow structures based on existing data sets. The main characteristics of this methodology, in comparison with previously existing ones, are its multi-scale and non-local character. The multi-scale nature, implemented by means of the curvelet transform, provides the framework for studying the evolution of the structures associated with the main ranges of scales defined in Fourier space, while keeping the localization in physical space that enables a geometrical study of such structures. We note that the multi-orientation decomposition included in the curvelet transform, not used in this study, can be useful when analyzing other flows in which the directionality of the structures can play a significant role, such as channel flow. The non-local character of the methodology is achieved through the calculation of area-based probability functions of the differential-geometry properties of the surface under consideration. It is also a generic methodology, not intended to educe a particular kind of geometry, but able to manage and classify all possible geometries. There are three main steps involved: extraction, characterization, and classification of structures. Individual structures (considered as closed surfaces disconnected from each other) are studied.

Results of its application first to a virtual world of modeled structures for system validation purposes and then to different fields obtained from DNS turbulence databases have been presented. From its application to the passive scalar fluctuation field advected and diffused in incompressible statistically stationary homogeneous isotropic turbulence in a 513^3 periodic box, the following conclusions can be drawn: first, the multi-scale decomposition resulted in a set of scalar fields (associated with the different ranges of scales extracted) with volumetric probability density functions of decreasing width for smaller scales. In addition, those probability density functions corresponding to scales approximately in the inertial range tend to overlap. Secondly, the study of the structures educed for the different scales shows a transition of their geometry from predominantly the blob-like and tube-like kind in the inertial range of scales toward sheet-like structures in the dissipation range. The dominant structures become more and more stretched for the smaller scales. This transition of geometry is smooth, complicating the automatic classification of structures. There are not clearly distinct groups of structures with a common geometry, but a continuous distribution of them filling the spectrum of present geometries instead. Thus, the application of the clustering algorithms is more challenging. In this case, three groups were educed automatically by applying the clustering technique implemented, and their projection in the visualization space and the identified cluster centers agree with the comments stated above. Nevertheless, clustering results are to be used with care in these conditions in which the points are so continuously distributed in the feature space used for clustering.

This methodology was then applied to the enstrophy and dissipation fields of a second database, obtained from a DNS of incompressible homogeneous isotropic turbulence decaying in time in a periodic box, at the time of maximum enstrophy of the flow. Three different grid resolutions were analyzed, corresponding to 256^3, 512^3, and 1024^3 points, with identical initial conditions and similar $Re_\lambda \approx 77$, resulting in $k_{\max}\bar{\eta}$ of approximately 1, 2, and 4, respectively. This allowed us to compare the geometry of the structures for different resolutions and evaluate whether the traditional DNS grid-resolution criterion $k_{\max}\bar{\eta} \approx 1$ is adequate for such geometrical analysis of the educed structures.

The 1024^3 case showed a continuous transition, for decreasing scale, from blob-like and moderately stretched tube-like structures at large scales to highly stretched sheet-like structures at the smallest scales under study. Intermediate scales of $\omega_i\omega_i$ show a dominance of tube-like structures, which is consistent with the presence of so-called 'worms' in previous studies (Siggia, 1981; Jiménez et al., 1993). Tube-like structures appear also at intermediate scales of $S_{ij}S_{ij}$ but in less proportion than for $\omega_i\omega_i$. The case with smallest grid resolution (256^3 points) did not capture the predominance of highly stretched sheet-like structures educed for the small scales at higher grid resolutions. This suggests the necessity to resolve sub-Kolmogorov scales for a proper geometrical study of the smallest structures of intermittent fields in turbulence, as was previously stated in the literature (see Shumacher & Sreenivasan, 2005; Horiuti & Fujisawa, 2008).

For the 1024^3 case, clustering techniques used during the classification step to obtain distinct groups of geometries among the educed structures resulted in three and two as the optimum number of groups obtained for $\omega_i\omega_i$ and $S_{ij}S_{ij}$, respectively. Blobs, tubes, and sheets can be seen as the predominant structures in the three groups of $\omega_i\omega_i$, while blobs and sheets are predominant in $S_{ij}S_{ij}$; but tubes, present also in this latter field, were included among the two optimum groups. Optimality scores for other number of groups did not differ substantially from the optimal results. This is a consequence of the continuous distribution of geometries, which indicates that the educed groups are not highly differentiated from each other and that the clustering results in this case should again be considered with reserve.

8.2 Assessment of non-local methodology complementing existing local identification criteria

We then applied the same non-local methodology for the study of the geometry of structures to two scalar fields, Q and $[A_{ij}]_+$, used by local criteria of identification of tubes and sheets in turbulence, based on the physical meaning of those quantities, that have been proposed in the fluid mechanics literature. This application confirmed the geometrical character expected for the majority of structures educed from those two fields (which before had been done only visually) by providing the necessary mathematical and geometrical background as well as means for quantifying the frequency of appearance of each geometry. Clustering techniques in this case provided a much clearer optimum number of two groups of structures, well differentiated. 96% of the structures of Q and $[A_{ij}]_+$ were assigned to separate groups by the clustering algorithm. Q structures were found to be mainly tube-like, while $[A_{ij}]_+$ were recognized as sheet-like. A small amount of structures of both fields present a geometry that does not correspond to the expected shape. For example, some tubes were found among structures of $[A_{ij}]_+$.

8.3 Proximity issues from a geometrical perspective

Finally, we introduced a new methodology for the study of proximity issues among structures corresponding to different fields, from a geometrical perspective. It provides information about the type of geometry found in structures of one group surrounding those of another, indicating the proximity and area coverage, by means of joint probability density functions. The set of surrounding structures can be also split into groups, and quantitative results for each group, concerning the proximity to the other structures, are shown by means of cumulative marginal probability density functions. The representation of the geometrical character of each structure is closely related to the visualization space used in the classification step of the previous study of the geometry of structures in turbulence (as introduced in Chapter 2). We applied this new technique to structures of Q, $[A_{ij}]_+$, $\omega_i\omega_i$ and $S_{ij}S_{ij}$, taken by pairs.

Structures of Q appear closely surrounded, partially overlapped and/or intersected by those of $[A_{ij}]_+$. Comparatively, other structures of Q appear farther from themselves and cover a smaller proportion of their area. A second group of proximal structures of $[A_{ij}]_+$ surrounds those of Q at a farther distance, comparable to the distances where other structures of Q are located, which they might be closely surrounding.

Considering only structures of $\omega_i\omega_i$ those extracted at an intermediate scale (predominantly tube-like) are surrounded primarily by $\omega_i\omega_i$ structures at the immediately smaller scale, and to a lesser degree by structures of even smaller scales. Structures of $\omega_i\omega_i$ at the same intermediate scale appear significantly farther. Two groups of surrounding geometries are dominant: sheet-like structures are closer; tube-like structures are farther but they cover a large proportion of the area of the structures they surround, thus indicating that the close sheet-like structures are not eclipsing them.

When $\omega_i\omega_i$ at the same intermediate scale are studied in relation to the structures of $S_{ij}S_{ij}$ at that and smaller scales, a more balanced contribution from all scales is observed. Sheet-like geometries are again the closest, and they appear to wrap around the tubes of $\omega_i\omega_i$, eclipsing more effectively other farther geometries.

8.4 Computational remarks

The requirements of our implementation and application of these methodologies to the 256^3 and 512^3 databases do not exceed the computational resources offered by a normal desktop or laptop computer. For the case of 1024^3 grid points, those steps involving Fourier transforms—computation of the fields in physical space from their spectral counterparts, spectral differentiation, and curvelet-based filtering during the multi-scale decomposition—required parallelization and the use of clusters of computers. The rest of the algorithms involved in both methodologies were designed to operate both in parallel and serial environments, independently of the size of the database. For serial operation, splitting and reconnecting algorithms were developed.

8.5 Future work

Both methodologies presented here could benefit from the addition of other geometrical and non-geometrical (e.g., physical) parameters in their analysis. The former could improve the characterization and classification of individual structures, while the latter could be used to relate geometrical properties of those structures with their own physical aspects or those of the surrounding structures. This potential for expansion was a driving criterion during the design and development of both methodologies, translated into the modular character of their implementation.

In the case of the methodology for the study of the geometry of structures, this modularity, consequence of its conceptual division into the three main steps of extraction, characterization, and classification, should facilitate future algorithmic improvements corresponding to each step. For example, the extraction step of the methodology for the study of the geometry of structures currently utilizes iso-surfaces of the (filtered component) scalar fields. Iso-surfaces are a natural first choice to educe structures from a three-dimensional scalar field, but add the dependence on a particular (set of) iso-contour value(s). In our implementation we use the mean of each field plus twice its standard deviation; for higher-contour values the educed structures showed similar geometries, implying a low sensitivity with the contour values, within a certain range. Note that, for extremely high contour values, the number of educed structures will be significantly reduced (only iso-surfaces in the vicinity of a few absolute maxima of the scalar field will be captured) and their geometries could change. Different techniques for the determination of optimum global contour values, such as percolation theory and Morse (critical points) discrete theory were explored in the context of this research. Additional techniques, such as region-based optimum contour values could be applied. Concerning the characterization stage, refined and faster future algorithms for the computation of curvatures of discretized surfaces could be easily implemented. Alternatives to the currently implemented K-means clustering algorithm, part of the classification step, such as *fuzzy c-means* clustering or *density-based* clustering, more oriented toward educing intermingled clusters without clear boundaries can be considered. Also, the addition of other relevant parameters in the clustering process may be useful to allow more separation in those cases where a continuous distribution of geometries is found.

Application to other flows, in particular those with a strong anisotropy, such as channel flow, would be useful, not only to study the geometries present in structures of those flows, but also to compare with homogeneous isotropic turbulence that has been object of this research, as a first canonical case of study. It would help determine whether common geometries in the small scales of turbulence exist. The exploration of the geometry of structures of those anisotropic flows would benefit from the multi-orientation capability of the curvelet transform, part of our current implementation for the extraction of structures. This capability has not been used in our present applications, for dealing with isotropic turbulence. We note that the mean scalar gradient imposed to the passive scalar field is responsible for some anisotropy in the passive scalar fluctuation field, in contrast with the velocity field that advects it. But due to the relatively weak anisotropy and the use of the passive scalar fluctuation field as the first simpler case to test the methodology, a multi-orientation decomposition was not applied to it.

A multi-orientation analysis could also be useful to study relative alignment among structures, both for isotropic and anisotropic flows. This multi-orientation decomposition can be applied in the extraction of the structures from the original field and then used in the methodology for the study of proximity issues among structures of different sets.

A natural line of expansion of this work is the study of the evolution in time of the geometry of educed structures, as well as the proximity issues presently investigated, both at the individual and composite level. This can be achieved by including a time tracker of structures as an additional module in both methodologies. This may facilitate the search for potential geometrical 'attractors' in a suitable feature space, as well as the development of models of (composite) structure-dynamics. Applications in the tracking and evolution in time of individual Lagrangian structures and their developmental geometry and interaction may also be useful.