Volume Puzzle: visual analysis of segmented volume data with multivariate attributes

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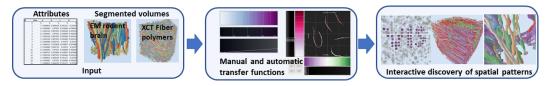


Figure 1: Inspired by word search puzzles, we present *Volume Puzzle*, a framework that allows us to interactively and/or automatically reveal spatial patterns from segmented volumes with associated multivariate attributes

ABSTRACT

A variety of application domains, including material science, neuroscience, and connectomics, commonly use segmented volume data for exploratory visual analysis. In many cases, segmented objects are characterized by multivariate attributes expressing specific geometric or physical features. Objects with similar characteristics, determined by selected attribute configurations, can create peculiar spatial patterns, whose detection and study is of fundamental importance. This task is notoriously difficult, especially when the number of attributes per segment is large. In this work, we propose an interactive framework that combines a state-of-the-art direct volume renderer for categorical volumes with techniques for the analysis of the attribute space and for the automatic creation of 2D transfer function. We show, in particular, how dimensionality reduction, kernel-density estimation, and topological techniques such as Morse analysis combined with scatter and density plots allow the efficient design of two-dimensional color maps that highlight spatial patterns. The capabilities of our framework are demonstrated on synthetic and real-world data from several domains.

Index Terms: Human-centered computing—Visualization—Visualization techniques—; Human-centered computing—Visualization—Visualization application domains—Scientific visualization

1 Introduction

The analysis of large 3D volumes composed of multiple objects with different shapes and characteristics is paramount for a variety of domains. Representative examples include:

- material engineering [2, 13], where high resolution tomographic scans are routinely used for investigation and diagnosis of samples in order to qualitatively and quantitatively analyze the characteristics of materials at micrometric or nanometric scale to understand whether they can be used for specific purposes like construction of photo-voltaic cells or electronic devices;
- physical simulations [11,25], where scientists analyze 3D static or dynamic volumes resulting from complex simulations related to various natural systems, like meteorology, or geology, or fluid interactions;

• neuroscience investigations [3, 10], where practitioners use high resolution acquisition of animal brain samples with the target of reverse engineering the connectivity between neurons.

In all these cases, the volume coming out of high resolution 3D imaging equipment or simulation data is typically segmented into objects associated with a variety of attributes that determine their characteristics. These attributes range from scalar values representing geometric, physical, or other domain-specific measures, to categorical labels identifying discrete or Boolean features.

The need to make sense of all this information has led to the development of visual analysis methods that couple attribute filtering schemes with real-time rendering to support sophisticated visual exploration [3, 4, 13]. As a general scheme, current methods couple the rendering of volumetric scenes incorporating domain knowledge with interactive tools to perform real-time culling of uninteresting data. However, the visual mapping between the attribute space and the 3D space remains a very difficult task, especially when the number of attributes does not allow for extensive exploration of the configuration space. To address these challenges, various methods have recently been proposed to simplify the analysis of the multivariate data in various contexts [18]. These methods strive to improve feature classification, fusion visualization, and correlation analysis. However, in several cases, domain scientists are interested in investigating whether objects with similar characteristics can form particular spatial patterns, like alignment, regular grids, or clustering (e.g., cells with similar characteristics in brain samples, or objects with similar size in material science samples).

In some cases, these spatial patterns are easily recognizable, especially when they are associated with visible geometric features, such bundles of fibers that have identical orientations (see Fig. 5). However, the most common cases include patterns that cannot be revealed, especially when they are related to complex combination of attributes. Accordingly, such investigations require reverse engineering efforts by the users through extensive attribute exploration and iterative transfer function editing. Selecting the right objects forming a pattern can be considered similar to solving word-search puzzles, in which the user must mark words hidden inside an array of letters. In this work, we propose a novel framework, dubbed Volume Puzzle, that aims to simplify the visual mapping of attributes to volumetric objects to support segmented volume analysis and discovery of spatial patterns. In particular, we strive to combine rapid identification of clusters in attribute space with the interactive 3D visual inspection of the arrangement of the identified objects in the 3D space. This workflow is supported by the combination of a real time ray casting of mipmapped label volumes, built on top

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of the Mixture Graph framework [4] with interactive methods for specifying one-dimensional and two-dimensional transfer functions that map scalar and categorical attributes to volumetric objects onthe-fly. The exploration of multivariate data is supported through a novel method for generating two-dimensional transfer functions, based on machine learning analysis of attribute space. In particular, we propose an algorithm that computes attribute projection through dimensionality reduction, kernel density estimation, and topological analysis based on the Morse-Smale complex. Although the attribute analysis components taken singularly are not novel, to the best of our knowledge, this is the first time they are combined together to reduce the complexity of attribute space and to produce automatic 2D transfer functions for interactive spatial analysis of segmented volumes with multiple attributes. We demonstrate the potential of our framework on a variety of synthetic and real world data from various domains. The explored data include label volumes obtained through segmentation of microscopy stacks representing material science samples and rodent brain samples at nanometric resolution. Our results show how our proposed semiautomatic transfer function method is able to reveal complex spatial patterns with minimal effort from the users.

2 RELATED WORK

Our work combines and extends the state-of-the-art solutions in interactive volume rendering of label volumes, multidimensional color mapping and transfer function, visualization of multivariate attributes, and the applications of Morse-Smale complexes in interactive visual analysis. Here, we review the methods most relevant to ours, referring the readers to well-established surveys on volume rendering [5], transfer functions [23], and multivariate spatial data visualization [18] for a wider coverage.

Multidimensional transfer functions In the literature, many sophisticated methods have been proposed to support volumetric exploration of complex data through the assignment of optical properties to voxel data [23]. In order to generate multidimensional transfer functions that can map multiple attributes to voxel color and opacity, Liu et al. [22] proposed a semi-automatic design system that represents high-dimensional data in the attribute space as a collection of low-dimensional linear subspaces. This collection is then used for creating multiple 2D views by projecting the embedded data points. While the proposed system works well for data with moderate complexity, it can become difficult to master once the attribute dimensionality grows, since the number of projected views becomes difficult to control. For this purpose, several space-based clustering methods have been designed to reduce the visual clutter during transfer function editing. The key idea of these methods is performing classification in high-dimensional feature space before transforming the volumetric data into a cluster space representation. This representation can then be easily explored by the user during transfer function editing [7,24]. This strategy has been exploited for automatic generation using different methods, such as intensity-gradient magnitude histogram [7], self-organizing map (SOM) to create transfer functions through a clustered 2D topology, and dendrograms for material segmentation and feature exploration [33]. Sharma et al. [31] proposed a fully-automated method based on the deduction of a material graph from material boundaries. However, this algorithm is best performing only on materials with well-separated interface edges, which is not the case with most real data. In this work, we propose a technique based on dimensionality reduction, density estimation and Morse-Smale analysis to provide a solution for addressing cluttered transfer functions.

Morse-Smale complex in Visualization Morse-Smale Complex is a topology analysis method that partitions a manifold or a scalar field according to the behavior of the gradient. This is performed in a way that all points in a partition are characterized by a

gradient which leads to the same critical point [16]. Lately, Morse-Smale complex has been applied on complex analysis in various domains, such as medical applications [33], where it has been used as a clustering algorithm for decomposing a 2D density plot into several valley cells. These cells represent potential structures within a scalar volume data. Gerber et al. [15] proposed a framework that combines topological and geometric information to generate simplified lower dimensional geometric representation of the Morse-Smale complex. The framework preserves important information about the high dimensional scalar fields and allows for interactive exploration of the input domain. The results have been demonstrated in different applications including physics, climate simulations, and combustion simulations [9, 12, 27]. Similarly, Abdelmula et al. [1] used dimension reduction and density analysis for spatial identification of prognostic tumor subpopulations on mass spectrometry imaging data. In the context of transfer function design for volume rendering, Kotava et al. [20] applied Morse-Smale complex for the analysis of 2D transfer functions related to standard magnitude-gradients in scalar volumes. We apply Morse-Smale theory to analyze 2D density functions in a reduced attribute space obtained through projection. In this sense, our approach has similarities with respect to methods proposed in Computer Vision for segmenting images based on density and topology analysis in the attribute space, where the pixel coordinates are also considered for increasing the dimensionality space [14,28]. We use the generated partitions to create automatic transfer functions for volumes which contain nominal data. This way, we provide an automatic method for exploring segmented volumes that enable the user to highlight spatial patterns.

Rendering of segmented volumes Segmented volumes are getting increasing popularity in various fields such as neuroscience, connectomics [17], and material science [35], where raw data is normally obtained by imaging through an electron microscope (EM) and segmentation techniques range from semiautomatic [10] to (almost) fully automatic [32, 36] approaches. To support real time exploration, hybrid strategies for ray casting have been recently proposed, that improve empty space skipping by balancing the computational load between the determination of empty ray segments (in the rasterization or object-order stage), and sampling of the nonempty volume data (in the ray-casting or image-order stage) [17]. This helps managing the culling of segments through a hierarchical representation of label sets that are leveraging on top of deterministic and probabilistic representations [6]. Recently, a data structure called Mixture Graph [4] has been proposed to speedup the rendering through the real time query of segmentation histograms. The Mixture Graph is based on the construction, factorization, and compression of mipmaps which contain convex combinations of segmentation IDs. This data structure enables the fast propagation of complex transfer function allowing for pre-filtered interactive rendering, and enabling real time query of partial histograms. In this paper, we build on top of the Mixture Graph approach, by exploiting the capabilities of multidimensional transfer function editing and adding automatic schemes based on attribute space exploration as well as density estimation and topology analysis.

3 METHODS









Figure 2: **Density-based automatic transfer function:** The computation pipeline (left to right) starts by attribute projection through dimensionality reduction, density-function computation through kernel density estimation, generating Morse-Smale complex manifolds, and finally performing the geodesic interpolation.

The *Volume Puzzle* framework is an interactive volume visualization system that works with segmented data, and in which every segment is associated with a list of attributes. We can formalize the representation of a segmented volume as a function $\lambda(\mathbf{x})$ assigning labels to voxel positions:

$$\lambda: D \subset Z^3 \mapsto L \subset Z \tag{1}$$

where D denotes the spatial domain as regular grid, and L is a set of labels representing the segments contained in the 3D space. Each segment λ is also characterized by an heterogeneous feature vector $\phi(\lambda)$ that can be represented as a function mapping each segment to a number S of scalar attributes and a number N of categorical attributes:

$$\phi: L \subset Z \mapsto R^S \times Z^N \tag{2}$$

3.1 Architecture overview

The proposed framework contains the following components:

- an interactive GPU volume renderer using ray casting and a specialized mipmapped representation of label volumes $\lambda(D)$ and based on the Mixture Graph data structure [4] (we refer readers to the original publication for technical details);
- interactive transfer function widgets for selecting attributes and specifying the optical properties of segments in the form of color and opacity for the accumulation during ray casting process, either monodimensional or bidimensional;
- semiautomatic 2D transfer function widgets for specifying segment color and attributes through the application of dimension reduction schemes, and topology analysis of the density function computed in the reduced attribute space.

Transfer function editing The assignment of the optical properties to segments consists of mapping colors and opacities to each segment λ that is represented inside the volume: $C = C(\lambda)$ and $\alpha = \alpha(\lambda)$. This could be done by selecting each segment singularly and assigning the optical properties one by one, or through functions that map individual or multiple attributes of the segments. Our system provides widgets for performing this manual specification by using single attributes: the user can select an attribute of interest to specify a colormap and an opacity function through an interactive design of a piecewise linear function. We also support bi-dimensional transfer function editing by providing a widget in which users can select two attributes, and create composite transfer functions that blend single-axis opacity functions (through multiplication), and single attribute colormaps (through interpolation). In order to guide users in the definition of the transfer functions, we provide a scatter plot of the object attributes. However, bi-dimensional transfer functions have the issue of a limited discrimination power that make them difficult to master for discriminating areas. Moreover manual selection of attributes can be a time consuming process, especially when the volume data contains a significant number of attributes.

3.2 Density-based Morse-Smale automatic transfer function

In order to speed-up the visual analysis process, we introduce an automatic method for aggregating multiple attributes together and generating an automatic transfer function based on density analysis. The method is composed of the following steps: dimension reduction of attributes in a way to project them to 2D space, computation of a density function over the projected parameter space, and topology analysis of the density function for highlighting critical points that are used for interpolating a 2D transfer function (see Fig. 2).

Dimension reduction Various methods can be considered for performing attribute projection, and users can select either to use all attributes or to choose a subset. In our preliminary tests, we considered Uniform Manifold Approximation and Projection (UMAP), that is based on the assumptions that data is uniformly distributed on

Riemannian manifold, and searches for a low dimensional projection of the data that has the closest possible equivalent fuzzy topological structure [26]. However, other methods for projecting attributes can be used and incorporated in the system, like Principal Component Analysis (PCA) [19] or t-Stochastic Neighbor Embedding (t-SNE) [21]. The projected space can be either used for the manual specification of the transfer function by editing opacity and color maps, or can be used for the density analysis.

Kernel density estimation Given N samples containing 2D attributes $\mathbf{x_k}$, either in the projected parameter space or in axis selected by users, a density function can be computed through the following estimator:

$$\delta(\mathbf{x}) = \frac{1}{N} \sum_{k=1}^{N} K\left(\frac{\mathbf{x} - \mathbf{x_k}}{h}\right),\tag{3}$$

where $K(\mathbf{x})$ is a kernel function, and h is a smoothing parameter called bandwidth [34]. Various choices of kernel functions can be considered: in our tests, we used the Gaussian normal kernel

$$K(\mathbf{x}) = \frac{1}{\sqrt{2\pi}} e^{-\frac{\mathbf{x}^T \mathbf{x}}{2}}.$$
 (4)

In this way, the process of recovering the density function $\delta(x)$ is similar to the concept of the mixture-of-Gaussians concept: it uses a mixture consisting of one Gaussian component per point, in a way that results an essentially non-parametric estimator of density.

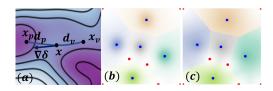


Figure 3: **Geodesic interpolation.** (a): for each sample x we compute a normalized geodesic interpolation factor by computing the geodesic distance from the peak and the valley in the same Morse-Smale partition through backward and forward integration of the gradient field. (b): example of geodesic interpolation. (c): examples of linear interpolation. Blued dots represent peaks of the Morse Smale Complex while red dots represent valleys.

Application of Morse theory The Morse theory is a powerful topology framework for the analysis of functions, since it provides tools for subdividing the domain according to the classification of critical points into partitions exhibiting gradient similarity. Moreover it can be used for generating natural interpolation fields in the attribute space by exploiting the gradient field and the inherent streamlines for performing geodesic interpolation. In our case, we computed a Morse-Smale Complex on top of the density function $\delta(\mathbf{x})$ [15] to identify the critical points. Then, we subdivided them into peaks and valleys/saddles. Next, we used the manifold partitions to drive geodesic interpolation in the attribute domain. Users can specify the desired optical properties by simply assigning the material properties for density peaks (colors C_p and opacities α_p) and valleys (in most of our results we put a neutral light color \hat{C}_{ν} for all valleys), and an additional 1D opacity function $\alpha(\sigma)$ based on a normalized geodesic interpolation factor σ that is computed as $\sigma = \frac{d_v}{d_p + d_v}$, where d_p and d_v are respectively the geodesic distances between the sample point x and the connected peak x_n and valley $\mathbf{x}_{\mathbf{v}}$ in the same partition (see Fig. 3.2 (a)). Hence, for each attribute sample **x** the material properties are: $C(\mathbf{x}) = \sigma C(\mathbf{x_p}) + (1 - \sigma)C(\mathbf{x_v})$ and $\alpha = \alpha_p \alpha(\sigma)$ The geodesic distances are obtained by computing the streamline passing through the sample point x: for doing that, we use the sample point x as seed, and we perform forward and backward gradient integration through 4th order Runge Kutta [30] in a way to reach the peak x_p and the valley x_v connected to x. The process is equivalent to the popular streamline integration method used in flow visualization, and provides us a way to compute a smooth automatic transfer function incorporating the topological features of the density map. Compared to standard linear interpolation, since it considers also valleys and gradient field, geodesic interpolation allow to obtain transfer functions separating more clearly the clusters originated around density peaks (see Fig. 3.2 (b) and (c)). In Sec. 4 we show how this transfer function can support the detection of spatial patterns in synthetic and real-world data.

4 RESULTS

We developed the VolumePuzzle in Python and C++, using OpenGL and GLSL for volume ray casting, and QT for the transfer function widgets. The attribute analysis methods are implemented through specific Python libraries, including UMAP or t-SNE for dimension reduction and kernel density estimation, and they are encapsulated in modules that communicate with the framework through a Python/C API wrapper interface. We performed a preliminary assessment of the capabilities of our framework on a variety of synthetic and real-world data from different domains. Since the method is applied inside the Mixture Graph framework, we currently deal with volumes containing segments on the range number 1K - 10K, and the underlying image space for attribute interpolation is 128x128, hence our current Python implementation is adequate for computing projections, and transfer functions in reasonable times for interactive analysis (few seconds for the overall automatic computation process).

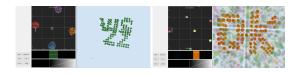


Figure 4: **Visual analysis of synthetic data:** two examples of test volumes containing spheres associated with scalar attributes. Only The automatic transfer function is able to highlight the spatial pattern.

Synthetic data For testing our system and the automatic transfer function approach, we generated a variety of synthetic examples (see Fig. 4). In these examples, the volume dataset is composed of K disconnected objects having identical spherical shape and size, and organized in a regular 3D grid with a little amount of jittering in the position, for a total number of 4096 segments on a $512 \times 512 \times 512$ grid. Each object is corresponding to a segment and is associated with a vector of S scalar attributes that we randomly generate according to normal distributions with different means and variances. Only a particular combination of them is able to solve the puzzle by revealing a visible pattern like a short writing or a simple shape (as visible in Fig. 4). In our preliminary tests, which are run with a variable numbers of attributes (between 4 and 10), we could assess that the standard 1D and 2D transfer functions were not able to reveal the patterns, while our semiautomatic transfer function approach allowed users to highlight them immediately (see supplementary video).

Real world data We carried out a preliminary evaluation on two real world datasets, namely from materials science and connectomics. The first one is an XRray CT scan of a sample containing Fiber-Reinforced Polymers, with $614 \times 961 \times 600$ voxel resolution and containing 15,917 segments, while the later is a nanometric resolution rodent brain sample extracted from hippocampus region, with $831 \times 831 \times 280$ resolution and a total number of 353 segments representing various neural structures [8]. For both datasets,



Figure 5: Visual analysis of XRay CT of Fiber-Reinforced Polymers: VolumePuzzle can support materials science experts for individuating spatial patterns in fiber organizations. Left: 2D transfer functions for highlighting patterns due to different orientations. Right: automatic density-based transfer function for highlighting patterns due to orientation or other geometric features (length, diameter).

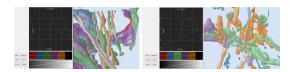


Figure 6: Visual analysis of SSEM rodent brain sample: VolumePuzzle can support neuroscience experts for individuating spatial patterns in neural structures, like axon bundles (left) or post-synaptic density formation (right).

we based our analysis on the following precomputed geometry attributes: length, diameter, and orientation components along the three axis directions. For the first dataset, a spatial pattern is originated by the different fiber orientations, while the other is originated according to different lengths of fibers (see Fig. 5): in both cases, both the manual and automatic transfer functions are able to reveal them, with the significant difference that the automatic transfer function reveals immediately the main patterns without the timeconsuming attribute search involving trial and error strategy. For the connectomics dataset, a preliminary assessment from a domain scientist highlighted that the framework is able to simplify visual analysis of unannotated segmented volumes, by clustering neural structures according to functional characteristics, like axons bundles and post-synaptic densities (see Fig. 6). Further investigation is needed to assess that the system can be used for automatic semantic labelling in connectomics.

5 Conclusions

We presented a framework for highlighting spatial patterns in segmented volume data based on multidimensional transfer functions using dimensionality reduction, density estimation and topology analysis for reducing the complexity of attribute space. The current implementation is limited to moderate complexity volumes in terms of number of segments: in order to scale over more complex volumes, concurrently with the revision of Mixture Graph data structure, we plan to consider more sophisticated GPU methods for dimension reduction [29], density estimation, MSC computation, and geodesic interpolation [14]. Moreover, since our target was the discovery of spatial patterns, we did not investigate how the nonlinear properties of various embeddings can affect the computation of the transfer function. As future work, together with an analysis of non-linear properties, we plan to extend the evaluation with user performance analysis, and with volume data coming from other domains. In particular, the framework can be adapted to work on multi-attribute scalar volumes or ensemble simulations by considering each attribute as a segment and each leaf voxel as a mixture (or histogram). To deal with scalability in image space, we plan to perform analysis on downsampled versions of the attribute space directly mapping to the volume mipmaps. Finally, we plan to investigate whether density-based attribute analysis can contribute to visual explainability of deep learning models.

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