Robust Topology-based Multiscale Analysis of Scientific Data

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Short Abstract/Introduction: *Hierarchical function decompositions and error driven simplifications might not ensure a precise control of topological features during multiscale analysis, impairing applications where topological control is more relevant than numerical approximation error. Topology-based multiscale analysis has emerged as an alternative to these conventional approaches, helping to understand complex scientific data.*

Multiscale analysis has emerged as one of the most effective representation mechanisms for exploring massive and complex data sets. Most methods devised for multiscale analysis, such as function decomposition using hierarchical basis and geometry based mesh decimation, rely on simplification mechanisms that attempt to minimize the numerical approximation error between models in consecutive levels of the hierarchy. Although numerical error driven multiscale methods are quite effective in a wide range of applications, the "blindness" for monitoring topological aspects renders such techniques inadequate for dealing with problems where the control of topological features and their spacial relationship are essential.

The search for topology-aware methods is not new, with initial ideas dating back to the 19th century [6]. However, much of the early research has been neglected, being rediscovered only recently when topology ceased to be a purely abstract mathematical concept, and became an important and computationally efficient data analysis tool. A sudden boost of topological tools has been motivated by current developments of robust combinatorial algorithms which replace previously existing techniques based on costly and unstable numerical integration methods. This change of paradigm has enabled the use of topological tools in large scale problems, making topology-based multiscale data analysis a feasible methodology.

The fundamental element in topological analysis is the detection and classification of the critical points of a function f. A point in the domain is critical if the gradient vanishes at that point, that is, $\nabla f(p) = 0$. Notice that ∇f points in the steepest ascending direction of f. One can classify critical points by the behavior of gradients in a small neighborhood around the point: At maxima, all gradients in the neighborhood point towards the maximum; At minima, all gradients point away from the minimum; and At saddles, there is a mixture of regions pointing towards and away from the saddle. Equivalently, one can classify critical points by the number and connectivity of regions in the neighborhood with lower and higher function values.

Critical points are crucial when analyzing f as they form the *start* and *end*-points of *integral lines.* Integral lines are paths that are everywhere parallel to the gradient of f and describe what is called the *gradient flow* of f. Therefore, removing critical points (in pairs) from f implies a re-routing of integral lines which, overall, results in a smoothing of (the gradient flow of) f. Consequently, removing critical points corresponds directly to a (local) simplification of f based on topological rather than geometric considerations. Similar to the geometric approach, this topological simplification leads naturally to a topology-based multiscale analysis of f driven by the successive removal of critical points.

Critical Points

Although an extensive description about critical points and related properties is beyond the scope of this article, we present in the following essential concepts that make up the basis of the robust topological multiscale analysis. We refer the interested reader to Munkres [8] and Milnor [7] for a mathematically precise description of the topological concepts we present only intuitively. A mathematically well founded presentation but with a good computational flavour can be found in the recent surveys [4, 1].

Morse functions

Morse theory provides the foundation for the majority of current techniques concerned with topological multiscale analysis. The key characteristic of Morse theory is the possibility of getting information on the topology of a domain by analyzing the critical points of a function defined on that domain. As already mentioned, given a smooth scalar function $f : M \subset \mathbb{R}^n \to \mathbb{R}$, the points where the gradient of f vanish characterize the critical points of f. A critical point p is non-degenerate if the determinant of the Hessian matrix (matrix of second partial derivatives) of f is not zero at p. A *critical value* is the real number corresponding to the image of a critical point by f. A function f is a *Morse function* when all its critical points are non-degenerate and have pairwise different function values. Morse functions admit only finitely many isolated critical points, moreover, these functions become extremely simple in the neighborhood of a critical point. More precisely, the Morse lemma states that any smooth function behaves as a quadratic form near a non-degenerate critical point: that is, it is possible to choose a local coordinate system such that $f(x_1, \ldots, x_n) = \pm x_1^2 \pm \cdots \pm x_n^2$ in this neighborhood. The number of minus signs in this equation defines the *index* of a critical point, and corresponds to the number of independent directions in which f decreases. For example, for Morse functions defined on two-dimensional domains, the indices of minima, saddles, and maxima are 0, 1, and 2 respectively.

The relationship between the critical points of f and the topology of its domain $\mathbb{M}$ is established by analyzing the changes in the *level sets*, the preimage in $\mathbb{M}$ of some scalar value t, $L(t) = \{x \in \mathbb{M} \mid f(x) = t\}$, as the parameter t changes. In fact, a strong mathematical result ensures that the topology of level sets only change when t passes through a critical value. Furthermore, the type of topological change, such as the creation/removal of tunnels or components, is intrinsically related to the index of the critical point. The utility of critical points motivates techniques for finding them.

Robust identification of critical points is not straightforward: while extrema can be detected as the endpoint of most integral lines, ensuring that each extrremum is found on no spurious extrema have been introduced requires combinatorial techniques. Furthermore, as discussed below, detection of saddle points is significantly more challenging. Consider, for example, the gravitational field between earth and moon, as depicted in Figure 1. Any particle released in the gravitational field follows an integral line towards a maximum located in either the earth or the moon. There is only one point in space, a saddle point, where a particle released at this location remains at rest. Detecting this saddle point is equivalent to finding an integral line with one endpoint being the saddle, computationally a very difficult task.

Functions occurring in scientific applications are rarely Morse functions, and mostly are available only as values at a finite set of sample locations, such as the vertices of a triangulation of the domain. Typically, a continuous function is recovered through interpolation. Piecewise linear interpolation, in particular, is often used with triangulated domains. Fortunately, the problem of detecting and classifying critical points becomes much more manageable for piecewise linear functions, using robust combinatorial methods.

Piecewise linear functions

Simplicial decompositions (triangulation in 2D and tetrahedralization in 3D) are one of the most popular domain discretization techniques. In this kind of representation, the domain is decomposed into a set of d-dimensional simplices, where 0,1,2, and 3 simplices are called vertices, edges, triangles and tetrahedra, respectively. It is convenient to assume that the function has pairwise different values at the vertices of each simplex. A continuous function is created by extending the function values through piecewise linear interpolation. Under these assumptions, critical points may occur only at the vertices of the simplices, making their identification easier.

In fact, in a piecewise linear function on a simplicial domain, critical points can be identified by analyzing the combinatorial structure of neighborhood of vertices. For example, if $f(q) < f(p)$ for all vertices q sharing an edge with p then p is a maximum. The lower link of p is the set of simplices spanned by the vertices q surrounding p. For a maximum, the lower link is a topological sphere. For a minimum, the lower link is empty. At a regular point the lower link is a topological disk and all other vertices are (multi-)saddles of various indices. As can be seen, in the piecewise linear case, all critical points can be identified and classified through a purely combinatorial analysis of the connected components of the lower link of each vertex (see Figure 2), thus introducing a very robust computational framework. An algorithmic description about critical point identification in three and higher dimensional domains can be found in [5] and [3], respectively.

Persistence

A crucial problem in data analysis is the assessment of the relevance of a feature. Measurement errors and discretization processes inherently add irrelevant features to data, making it difficult to discern vital features from all others. From a topological point of view, features are characterized by topological changes in level sets of the function, which, in turn, are intimately related with the critical points of the function.

We illustrate the relationship between topological features and critical points by examining the behavior of level sets in a sweep through the range of the function. Given a function f (Morse function) defined in a piecewise linear domain $\mathbb{M}$, one can sort the vertices of $\mathbb{M}$ in ascending order as to f. The vertex ordering allows to sweep $\mathbb{M}$ from the extremum minimum towards the highest maximum, identifying the occurrence of new feature each time a critical point is crossed. For example, consider a surface endowed with the height function, as illustrated in Figure 3. It can be seen that a new level set component is created as a consequence of starting to sweep the surface from the lowest minimum. When the sweeping process reaches the next critical point, also a minimum, a second level set component is created. Both these components are features. The first and second features stay "alive" until a new critical point is reached, a saddle point now, which merges the two existing features into a single one, effectively "destroying" one of the features. Creation, splitting, or merging of features happens each time a critical point is crossed, ending only when the sweep crosses the highest maximum.

The process described in the example above is usually called *filtration* and it provides a natural mechanism for pairing critical points in accordance with the "birth" and "death" of features, that is, one can build critical pairs (p_i, p_j) indicating that a new feature is created in $f(p_i)$ and destroyed when the filtration crosses $f(p_j)$. The pairing of critical points allows to measure the relevance of a feature by for example comparing the function values in each critical point. In more mathematical terms, one can compute the relevance of feature represented by (p_i, p_j) through $\mathcal{P}_i^j = |f(p_i) - f(p_j)|$. The relevance of a feature is usually called *persistence*, a concept that enables to rank features and build hierarchies, an essential component of multiscale analysis.

Once each pair of critical points represents the birth and death of a feature, the removal of a critical pair represents the removal of a feature, thus resulting in a simplification of the data. In a multiscale analysis, critical pairs are withdrawn according to their persistence, meaning that the smaller the persistence of a critical pair is the earlier that pair is removed. The models on the right of Figure 3 illustrates the above mechanism applied to a 3D model. Notice, that the removal of the critical pair formed by the left minimum and the lowest saddle point makes the "left leg" of the model disappear, whereas the removal of the critical pair formed by the two other saddle points cause the tunnel to be filled. The resulting model is a simplified version of the original one, as it contains a smaller number of features, that is, the simplified model is in a "coarser" scale than the original surface. A detailed description about persistence and corresponding properties can be found in [2].

The aforementioned framework has been employed in a wide class of applications, making possible to handle problems where conventional approaches are not effective. Some examples of such applications are discuss in the following.

Applications

Analysis and Multi-Scale Representation of Surface Meshes

One application of critical points in geometric modeling is finding and highlighting defects in geometric models. Pascucci et al. [**?**] developed a technique for automatically detecting defects in surface models by identifying saddles that create and destroy a loop. Ideally, a perfect mesh would only have “holes” where actual features are, such as the loops created by the arms and legs of the statue of David in figure 4. In practice, however, a mesh aquired from triangulation of points from a scan of the object can admit small holes or filpped triangles that can be very difficult to detect. By using critical points to find such defects, one can find small manifold handles and tunnels, not only non-manifold or missing triangles. The former defects are global in nature and therefore much harder to identify than the latter which can be found by checking a local neighborhood.

For each model, all saddle-saddle pairs are found that form a loop. The loop count is plotted above a certain persistence (as a percentage of function range) creating one-dimensional graphs, see figure 4. These plots indicate both the topological complexity of a model as well as a threshold separating noise from features. In particular, consider the David model: although not visible in traditional rendering, several tunnels exist in the model. These “noise” tunnels show up as low-persistence pairs in the plot. While these tunnels might not impact the visual quality of the model, they will adversely effect most geometric processing, e.g. simplification or parametrization of the surface. Automatic and robust identification of such defects is essential for applications that utilize manifold properties of a mesh.

Analysis of Porous Media

Next, we examine how critical points can be used to identify features at multiple scales in a volumetric simulation. Aerogels have recently become popular for their high insulating ability and low weight, motivating further research in material sciences. Gyulassy et al. [**?**] showed how critical points could be used to aid in understanding properties of such a material. In the simulation, a copper foam targeted for use as an insulating material for spacecrafts is hit by a micrometeoroid travelling at 5km/s. The following questions were of particular interest: How can one quantify the loss of porosity of the material? How does the filament density profile of the material change? What is the portion of the material that is affected by the impact crater? How does the structure around the impact crater change?

To answer these questions, Gyulassy et al. used a multi-scale representation of the topology of the data to explicitly extract the core structure of the filaments. The multi-scale representation was useful in eliminating confounding noise from the analysis. First, critical points of the function were identified. The 2-saddle-maximum pairs of this function correspond to the features of interest in this data, since the integral lines connecting them trace out the core structure of the filaments. Figure 5 illustrates the process of identifying critical points, distinguishing between features and noise, filtering and simplifying the topology, and finally using the extracted core structures to answer the motivating questions about the filaments.

Without direct control over the topological features, such analysis would be very challenging. While visual inspection of the simulation can give a general feel for how the filaments are affected by the impact of the micrometeoroid, examination of the core structures immediately reveals with a high degree of confidence the locality of the impact. The loss of porosity of the material becomes quantifiable by computing the length and number of cycles in the structure defined by the core lines. Finally, using critical points and persistence to reveal the stable underlying features of the dataset proved to be an essential tool for comparison of core structures at different time steps in the simulation.

References

[1] S. Biasotti, L. De Floriani, B. Falcidieno, P. Frosini, D. Giorgi, C. Landi, L. Papaleo, and M. Spagnuolo. Describing shapes by geometrical-topological properties of real functions. *ACM Comput. Surv.*, 40(4):1–87, 2008.

[2] D. Cohen-Steiner, H. Edelsbrunner, and J. Harer. Stability of persistence diagrams. *Discrete Comput. Geom.*, 37:103–120, 2007.

[3] H. Edelsbrunner and J. Harer. Jacobi sets of multiple morse functions. In F. Cucker, R. DeVore, P. Olver, and E. Sueli, editors, *Foundations of Computational Mathematics*. Cambridge Univ. Press, 2002.

[4] H. Edelsbrunner and J. Harer. Persistent homology - a survey. In J. E. Goodman, J. Pach, and R. Pollack, editors, *Surveys on Discrete and Computational Geometry. Twenty Years Later*, volume 453, pages 257–282. Amer. Math. Soc., 2008.

[5] A. Gyulassy, V. Natarajan, V. Pascucci, and B. Hamann. Eficient computation of morse-smale complexes for three-dimensional scalar functions. *IEEE Trans. on Visualization and Computer Graphics*, 13(6):1440–1447, 2007.

[6] J.C. Maxwell. On hills and dales. *The London, Edinburgh and Dublin Philosophical Magazine and Journal fo Science*, XL:421–427, 1870.

[7] J. Milnor. *Morse Theory.* Princeton Univ. Press, 1963.

[8] J.M. Munkres. *Elements of algebraic topology.* Benjamin/Cummings, 1984.

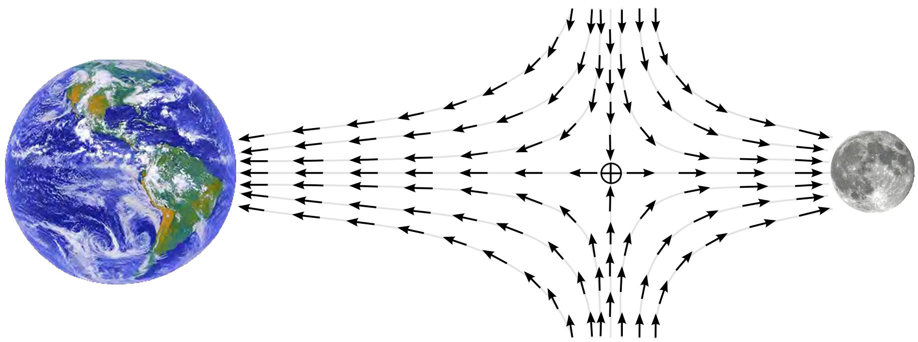

Figure 1: This is where a cool motivational picture should go

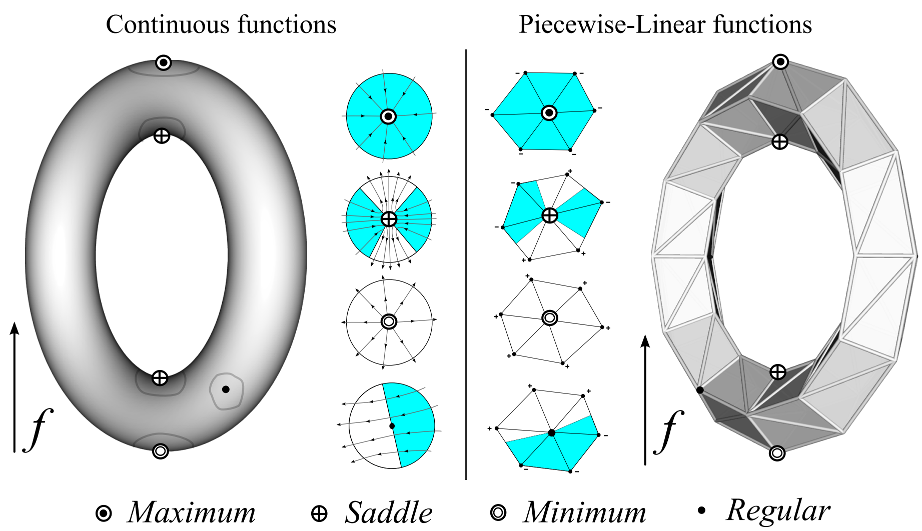

Figure 2: Critical points of a continous Morse function on a two-dimensional domain (left) include maxima, saddles, and minima. The gradient behavior (show with arrows) in a neighborhood around a critical point determines its classification. Regions in the neighborhood of a point with lower function value, called *oceans*, are colored blue, and regions with higher value, called *continents*, are colored white. The shape and connectivity of oceans and continents identify the type of critical point. At a maximum, the gradient points inwards everywhere, and correspondingly, its entire neighborhood is an ocean. At a saddle, integral lines approach from two directions and then diverge, creating two oceans and two continents. At a minimum, the gradient points away in the entire neighborhood, and correspondingly, the entire neighborhood is a continent. The gradient is non-zero at a regular point, and there is exactly one ocean and one continent. In a piecewise linear (PL) function (right), gradients are not continuous, and therefore critical points are identified using the shape of the oceans and continents in a 1-neighborhood around a vertex. The "+" and "−" signs indicate vertices that are higher or lower than the vertex in the middle. For the case of two-manifold domains, it is sufficient to count the number of continents and oceans around a vertex: maxima = 0,1; saddles = 2,2; minima = 1,0; regular points = 1,1.

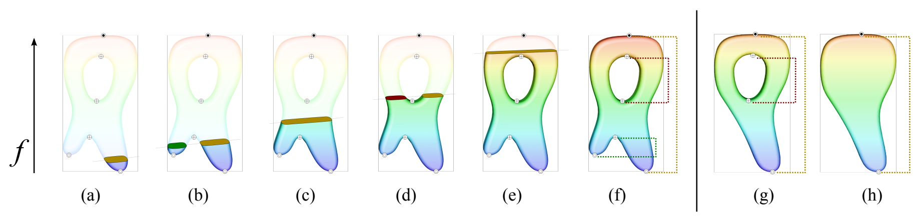

Figure 3: Displayed is a three-dimensional model with a height function. In a sweep from low to high function value, the level sets change their topology as various critical points are passed. (a) Passing the lowest minimum, a level set component (beige disk) is created. (b) The next minimum creates another level set component (green disk). (c) Passing the saddle “destroys” the most recently created (green) component, and the level set has only one connected component again. (d) Another saddle splits the level set and creates a new (red disk) contour. (e) The next saddle destroys this (red disk) contour, and (f) finally, the maximum destroys the level set component created by the first minimum (beige disk). The critical points that create and destroy a feature are paired. Subsequent removal of these pairs in order of persistence smooths the function by first removing a bump (g), and finally removing a tunnel (h). In this manner, removal of critical points gives direct control over simplification of a function for multi-scale analysis.

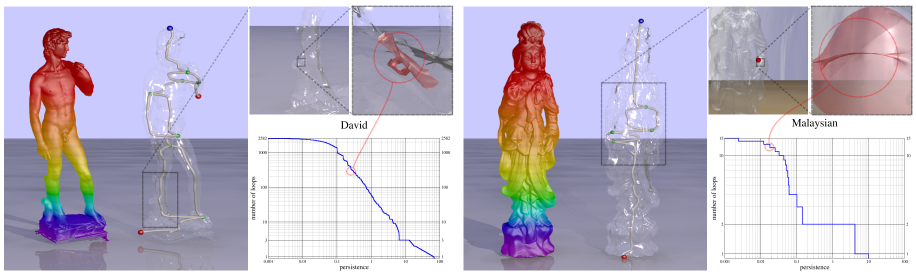

Figure 4: Surface meshes constructed from high resolution scans often have defects that are not visibile, however can be problematic for applications such as simplification or parametrization of the surface. In particular, the surface can have small manifold tunnels (defects) which are not detectable by local techniques. Here, we apply a height function to the mesh, and strong results from Morse theory guarantee that each tunnel will necessarily have a pair of saddles that create and destroy the feature. Two models are examined: (left) the the model of David has three main "holes", formed by each arm and the legs. Further investigation reveals that small "noise" loops also exist, defects. The plot shows the number of loops versus the simplification threshold. As in figure 3(g), cancelling a saddle-saddle pair removes these small loops. When the persistence threshold for simplification reaches $\tilde{1}0$, the plot flattens out, at which point only the 3 "feature" loops have not been removed from the model. This process is repeated (right) for the model of the Malaysian goddess. Again, the plot shows that there are exactly two "feature" loops. In both cases, the locations of the paired saddles pinpoint the defects in the surface meshes.

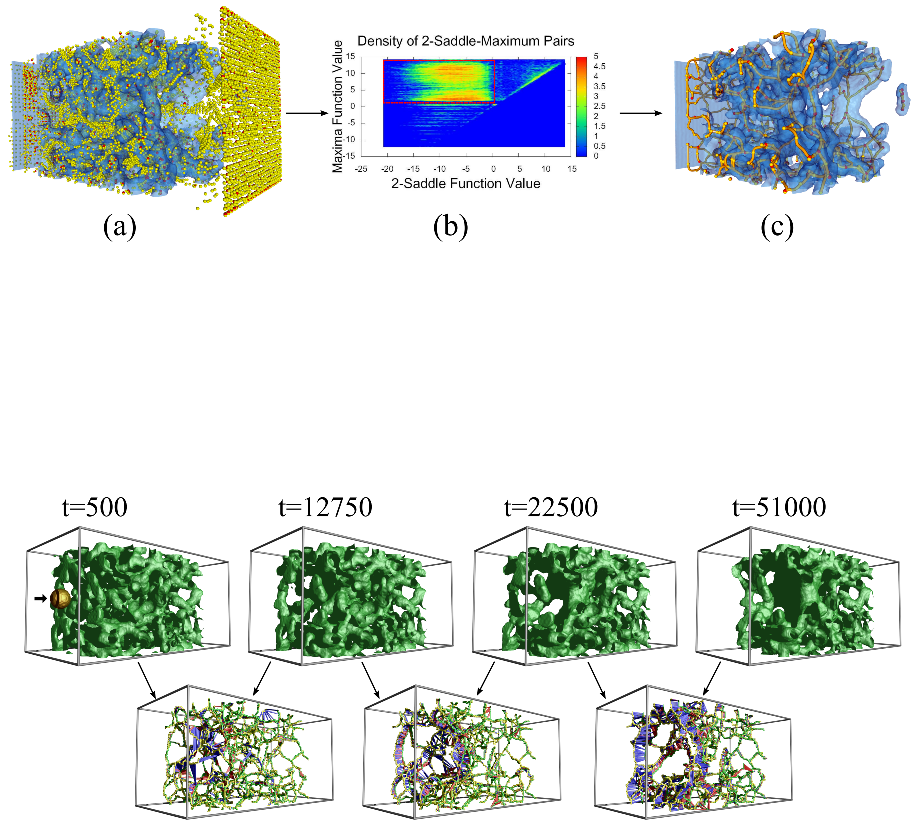

Figure 5: The critical points of a simulated porous solid are identified and used to extract features (top). In this experiment, the desired feature is the core structure of the filaments. The integral lines of 2-saddle-maximum pairs in this three-dimensional function form the core structures, however, due to noise and uncertainty in the simulation, there are initially many extra critical points (a). The 2-saddle-maximum pairs are displayed in a density plot (b), where color indicates the number of pairs in each bin. Distance from the diagonal corresponds to the persistence of a pair. Critical points are canceled in order of persistence, however, the simplification is guided using *filters*, explicit restrictions placed on the changes allowed to the topology by the cancellation of a critical point pair. In particular, various parameters used in the simulation indicate certain ranges of the 2-saddle and maximum values that correspond to imporant features. This plot inticates thresholds to select those features in the most stable manner possible, enabling removal of noise while preserving features. A stable core structure is identified (c) in this manner. The same filters and simplification is applied to extract consitent core structures for various timesteps as the simulated material is hit by a micrometeoroid (bottom). By inspecting the different core structures, changes in the connectivity of the material become obvious, and the loss of porosity can be quantified and computed.