Topological Analysis of Ensemble Scalar Data with TTK

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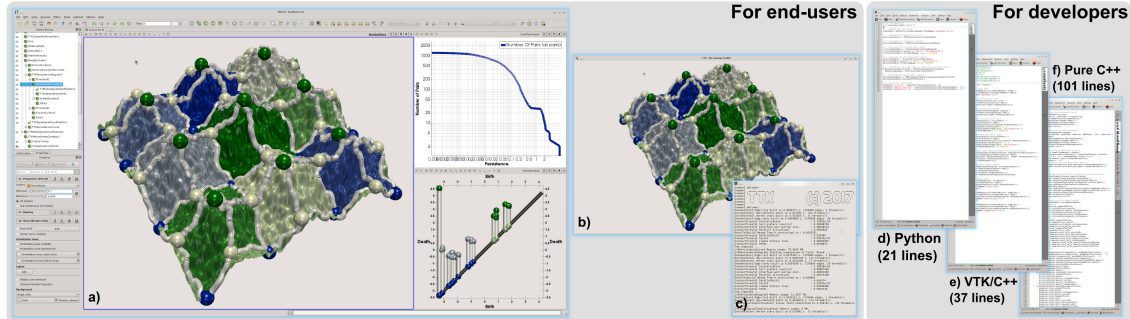
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Figure 1: TTK is a software platform for topological data analysis in scientific visualization. It is both easily accessible to end users (ParaView plugins (a), VTK-based generic GUIs (b) or command-line programs (c)) and flexible for developers (Python (d), VTK/C++ (e) or dependence-free C++ (f) bindings). TTK provides an efficient and unified approach to topological data representation and simplification, which enables in this example a discrete Morse-Smale complex (a) to comply to the level of simplification dictated by a piecewise linear persistence diagram (bottom-right linked view, a). Code snippets are provided (d-f) to reproduce this pipeline.

1 LEVEL OF THE TUTORIAL

This tutorial is targeted at a *Beginner* to *Intermediate* audience.

2 POTENTIAL SCHEDULE CONFLICTS

If possible, we would like to avoid any scheduling overlap with IEEE LDAV 2021 (which should take place on October 25). Coauthor Tierny is a cochair of LDAV this year, and many of the speakers, as well as the potential attendees, are members of both communities.

3 ABSTRACT

This tutorial presents topological methods for the analysis and visualization of scientific data from a user's perspective, with the Topology ToolKit (TTK), an open-source library for topological data analysis. *In particular, this year's tutorial has a special focus on ensemble data analysis with TTK.* Topological methods have gained considerably in popularity and maturity over the last twenty years and success stories of established methods have been documented in a wide range of applications (combustion, chemistry, astrophysics, material sciences, etc.) with both acquired and simulated data, in both post-hoc and in-situ contexts. This tutorial provides a beginner's introduction to topological methods for practitioners, researchers, students, and lecturers, with a special emphasis towards ensemble data analysis. In particular, instead of focusing on theoretical aspects and algorithmic details, this tutorial focuses on how topological methods can be used in practice to reduce ensemble datasets into concise yet meaningful topological data representations and how these representations can support advanced analysis. The tutorial describes in detail how to achieve these tasks with TTK. In comparison to the last iterations of this tutorial [14, 15, 17] (the 2020 edition video recordings are fully available online [15]), this iteration focuses on the practical usage of TTK for ensemble data analysis. First, we provide a general introduction to topological methods and their application in data analysis, and a brief overview of TTK's main entry point for end users, namely ParaView, will be presented. Second, we detail TTK's software infrastructure for ensemble data analysis, including TTK's Docker support (to facilitate its deployment on

computing servers), a tour of the topological data representations supported by TTK, TTK's python support and lastly TTK's cinema support (to manipulate ensemble of topological data representations with a database formalism). Third, we will present concrete use cases of ensemble data analysis and visualization, using contour tree alignment, mandatory critical points and ensemble clustering and summarization with persistence diagrams. Presenters of this tutorial include experts in topological methods, core authors of TTK as well as active users, coming from academia and industry. This tutorial mostly targets students, practitioners and researchers who are not necessarily experts in topological methods but who are interested in using them in their daily tasks. We also target researchers already familiar to topological methods and who are interested in using or contributing to TTK. We kindly ask potential attendees to optionally pre-register at the following address, in order for us to reach out to them ahead of the tutorial with information updates (for instance, last minute updates, instructions for the download of the tutorial material package, etc.): https://forms.gle/Me4mqYmJYJsgEQYU9 Tutorial web page (including all material, TTK pre-installs in virtual machines, code, data, demos, video tutorials, slides, etc): https://topology-tool-kit.github.io/ieeeVisTutorial.html

4 TUTORIAL ORGANIZATION

Online organization Since IEEE VIS 2021 will be an online event again this year, the TTK tutorial would also be organized remotely if this proposal was accepted. In particular, we would build upon our experience of 2020, for which we pre-recorded all the material for later re-use by the participants [15]. For this, we would be happy to adapt our organization to the technical recommendations from the IEEE VIS organizers (for instance, with pre-registration, talk pre-recording, online discussions with Discord, YouTube broadcasting).

Motivations Topological analysis techniques [29, 40, 47] have shown to be practical solutions in various contexts: isosurface extraction [7, 41, 53], feature tracking [44], volume rendering [57], data simplification [36, 51] and compression [45], similarity estimation [16, 43, 52, 54], geometry processing [48, 55] or data science [8, 10, 12]. They enable the concise and complete capture of the structure of the input data into high-level *topological data representations* such as contour trees [6, 21–23], Reeb graphs [24, 38, 39, 50], or Morse-Smale complexes [11, 26, 27]. Successful applications

in a variety of fields of science have been documented (combustion [4,25,32], fluid dynamics [5,9,30], material sciences [18,28,34], chemistry [2,19,37], and astrophysics [42,46]), which further demonstrates the importance of these techniques. While reference textbooks have been published [13], topological methods have not yet been widely adopted as a standard data analysis tool. We believe one of the reasons for this is the lack of open-source software that implement these algorithms in a generic, user-friendly, and efficient way. The Topology ToolKit (TTK) [3, 35, 49] has been released (BSD license) to fill this gap and 16 institutions have contributed to its development so far. Since it release in 2017, TTK's website collected 290k page-views, from 32k visitors. This indicates that a user base exists and that further efforts towards the explanation of TTK's usage would be beneficial to the community.

Target audience This tutorial targets beginners, students, practitioners, and researchers who are not experts in topological methods. It also targets researchers already familiar to topological methods and who are interested in using TTK for ensemble data analysis.

Tutorial goals The goals of this tutorial are to present the key tools in topological data analysis (the Persistence diagram, the Reeb graph and its variants, the Morse-Smale complex, etc.) and how they can be used in practice for ensemble data analysis. All examples will be illustrated with TTK. We expect participants to become capable of using TTK with ParaView independently, after attending the tutorial.

Hands-on material A large part of the tutorial will be dedicated to detailed example demos that the participants will be invited to reproduce. We will provide a rich material package including TTK pre-installs in virtual machines, (to be used by attendees during the tutorial), example ensemble datasets, demos, etc. Most of this material is already available on TTK's website [14, 17]. Our idea is that participants with a laptop will be able to follow along, regardless of their native OS. Attendees who attend just to listen and learn will receive sufficient material to try our examples at home.

Optional pre-registration In previous editions, we observed that attendees would benefit from having time before the tutorial to install materials and have their systems set up with the hands-on material. If our proposal is accepted, we will use the following on-line form (https://forms.gle/Me4mqYmJYJsgEQYU9) to notify audiences of where and how to download the material and build a mailing list to help form an informal community for the tutorial.

Proposal strengths In contrast to previous tutorials on topological methods [56], we believe this proposal to have a unique concrete and applicative appeal, by its focus on the *usage* of topological methods rather than on their *foundations*. Thus, we expect it to attract a larger audience than the specific subset of IEEE VIS attendees typically found in traditional topology sessions. Moreover, in comparison to the previous editions of this tutorial, this year's edition will have a special emphasis on ensemble data analysis, to exemplify TTK's features on a focused topic. We believe that the list of presenters is also a strength of this proposal. First, it includes topology experts as well as core developers and users of TTK. More importantly, it includes researchers with a variety of experience profiles (Ph.D. students, post-docs, professors) and backgrounds (industry, academia), which will ease interactions with a potentially heterogeneous audience. Moreover, the particularly large number of presenters has two merits. First, it imposes a mini-symposium structure, where speakers will give presentation lasting between 10 and 20 minutes, which will result in a lively rhythm in the overall tutorial. Second, this large number of presenters will be instrumental during the hands-on exercises, as there will be enough presenters such that one presenter can assist a small group of attendees (typically 3 to 4). Finally, we believe the detailed program of the tutorial (see Sect. 4) achieves a balance between concepts and concrete examples.

Detailed content The tutorial is divided into three main parts (each part being subdivided into modules), for a target duration of approximately 3 hours and a half. These three groups of modules can be organized differently to to fit any standard structure for breaks to match the tutorial schedule of IEEE VIS. After the tutorial concludes, we will make all content available from our website.

A. Preliminaries (70 minutes)
A1. General introduction *(10 minutes, by Julien Tierny)* This talk will provide an overview of the tutorial and discuss how concise topological data signatures can be used to reduce large-scale ensemble data, and still enable advanced analysis.
A2. Introduction to topological methods for data analysis *(30 minutes, Bei Wang)* This talk will present the core tools in topological data analysis (critical points, persistence diagrams [13], Reeb graphs and their variants [6, 22–24, 39, 50] and Morse-Smale complexes). In particular, it will detail how these tools can be used for data segmentation and feature extraction.
A3. Introduction to ParaView *(30 minutes, by Charles Gueunet)* This talk will provide a brief description of ParaView's main interface [1], in order to support its usage for beginners in the rest of the tutorial. This will cover the usage of filters, pipeline design, view manipulation, and Python exports as well as a quick introduction to Catalyst (for in-situ computations).

B. TTK infrastructure for ensemble data analysis (75 minutes)
B1. Running TTK with Docker *(15 minutes, by Christoph Garth)* This talk will describe how to use TTK with Docker, which is a typical solution for deploying TTK on high-performance infrastructures (for the in-situ computation of topological signatures).
B2. A tour of TTK *(30 minutes, by Joshua Levine)* This talk will provide an overview of the topological signatures supported by TTK and will illustrate how to apply them on concrete examples.
B3. TTK Python support *(15 minutes, Lutz Hofmann)* This talk will present how to deploy (with its Anaconda package) and use TTK in a Python environment with simple examples.
B4. TTK Cinema support *(15 minutes, Jonas Lukasczyk)* This talk will introduce TTK's Cinema support for storing and manipulating databases of topological signatures representing an ensemble.

C. Ensemble processing with TTK (70 minutes)
C1. Contour tree alignment *(15 minutes, by Florian Wetzels)* This talk will introduce the contour tree alignment module of TTK [33], which enables the simultaneous and coherent planar layout of an ensemble of contour trees (representing an ensemble dataset) for visual inspection purposes.
C2. Mandatory critical points *(15 minutes, by Julien Tierny)* This talk will introduce the mandatory critical point module of TTK [20], which enables the representation of the topological structures (join trees and split trees) which are common to all the members of the ensemble, to identify recurring features throughout the ensemble.
C3. Distances, barycenters and clusters *(15 minutes, by Jules Vidal)* This talk will show how to efficiently compare and cluster the members of an ensemble based on their persistence diagram [54].
C4. Ensemble summarization with linked planar views *(15 minutes, by Pierre Guillou)* This talk will show step-by-step how to generate, with multidimensional scaling, planar summarizations of the input ensemble, where each member is represented as a point in 2D and where similar members (in terms of their topological signatures) are projected in similar locations. Linked views, related to each point of the summarization, enable the visual inspection of each topological signature. Together, the planar summarization and its detailed linked view enable the visual analysis of global trends in the ensemble.
C5. Concluding remarks *(10 minutes, Julien Tierny)* This talk will conclude the tutorial and discuss perspectives and current efforts.

5 BACKGROUND AND CONTACT INFORMATION

Christoph Garth – *garth@cs.uni-kl.de* – is a professor of computer science at Technische Universität Kaiserslautern, and head of the scientific visualization group there. His research interests encompass the visualization and analysis of large scale data sets using methods from topological analysis, feature extraction, visual analytics, and high-performance computing, among others. In this context, he has

employed TTK in teaching, to provide students with an in-depth understanding of topological methods, as well as for his research, as a robust and mature basis to develop novel visualization algorithms.

Charles Gueunet – *charles.gueunet@kitware.com* – is currently an R&D engineer at Kitware. He received his PhD from Sorbonne Université (Paris, France) in 2019. He worked on high performance topological data analysis using level-set based abstractions. He is the author of several contour tree and Reeb graph modules in TTK.

Pierre Guillou – *pierre.guillou@sorbonne-universite.fr* – is a research engineer at Sorbonne University. He received his PhD from Mines ParisTech in 2016. He is an active contributor to TTK and the author of many modules created for the VESTEC project.

Lutz Hofmann – *lutz.hofmann@iwr.uni-heidelberg.de* – is currently a PhD student at Heidelberg University, where he received master's degrees in mathematics as well as in computer science in 2017. His research interests include feature-based visualization of higher-dimensional as well as time-dependent fields. He is the creator and maintainer of the Python Anaconda package of TTK.

Joshua A. Levine – *josh@email.arizona.edu* – is an associate professor in the Department of Computer Science at University of Arizona. Prior to starting at Arizona, he was an assistant professor at Clemson University, and before that a postdoctoral research associate at the University of Utah's SCI Institute. He received his PhD from The Ohio State University. His research interests include visualization, geometric modeling, topological analysis, mesh generation, vector fields, performance analysis, and computer graphics.

Jonas Lukasczyk – *jl@jluk.de* – is currently a staff scientist at the Technische Universität Kaiserslautern, at which he also obtained his PhD in 2019. His work focuses on Topology-Based Visual Analytics of Large-Scale Simulations. Several of his approaches use TTK as a backbone for reliable and reproducible data analysis.

Julien Tierny – *julien.tierny@sorbonne-universite.fr* – received the Ph.D. degree in Computer Science from Lille 1 University in 2008 He is currently a CNRS permanent research scientist, affiliated with Sorbonne Universite. Prior to his CNRS tenure, he held a Fulbright fellowship (U.S. Department of State) and was a post-doc researcher at the SCI Institute at the University of Utah. His expertise includes topological data analysis for scientific visualization. He is the lead developer of the Topology ToolKit (TTK).

Jules Vidal – *jules.vidal@sorbonne-universite.fr* – is a Ph.D. student at Sorbonne Universite. He received the engineering degree in 2018 from ENSTA ParisTech. His notable contributions to TTK include the efficient and progressive approximation of distances, barycenters and clusterings of persistence diagrams [31, 54].

Bei Wang – *beiwang@sci.utah.edu* – is an Assistant Professor in the School of Computing and a faculty member in the Scientific Computing and Imaging (SCI) Institute, University of Utah. Her research expertise lies in the theoretical, algorithmic, and application aspects of data analysis and data visualization, with a focus on topological techniques. In particular, her research leverages topological data analysis, which provides a strong basis for transforming large, complex data into compact, structure-highlighting representations.

Florian Wetzels – *f_wetzels13@cs.uni-kl.de* – is a PhD student at the Scientific Visualization Lab at TU Kaiserslautern. Previously he did his Master Studies in Computer Science at TU Kaiserslautern. His work focuses on algorithms and techniques in scientific visualization as well as in computational biology. Through his work on Contour Tree Alignmnents he became a contributor for TTK.

ACKNOWLEDGMENTS

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