

Geometric Detection Algorithms for Cavities on Protein Surfaces in Molecular Graphics: A Survey

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Abstract: Detecting and analysing protein cavities provides significant information about active sites for biological processes (e.g. protein–protein or protein–ligand binding) in molecular graphics and modelling. Using the three-dimensional (3D) structure of a given protein (i.e. atom types and their locations in 3D) as retrieved from a PDB (Protein Data Bank) file, it is now computationally viable to determine a description of these cavities. Such cavities correspond to pockets, clefts, invaginations, voids, tunnels, channels and grooves on the surface of a given protein. In this work, we survey the literature on protein cavity computation and classify algorithmic approaches into three categories: evolution-based, energy-based and geometry-based. Our survey focuses on geometric algorithms, whose taxonomy is extended to include not only sphere-, grid- and tessellation-based methods, but also surface-based, hybrid geometric, consensus and time-varying methods. Finally, we detail those techniques that have been customized for GPU (graphics processing unit) computing.

Human Factors in Streaming Data Analysis: Challenges and Opportunities for Information Visualization

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Abstract: Real-world systems change continuously. In domains such as traffic monitoring or cyber security, such changes occur within short time scales. This results in a streaming data problem and leads to unique challenges for the human in the loop, as analysts have to ingest and make sense of dynamic patterns in real time. While visualizations are being increasingly used by analysts to derive insights from streaming data, we lack a thorough characterization of the human-centred design problems and a critical analysis of the state-of-the-art solutions that exist for addressing these problems. In this paper, our goal is to fill this gap by studying how the state of the art in streaming data visualization handles the challenges and reflect on the gaps and opportunities. To this end, we have three contributions in this paper: (i) problem characterization for identifying domain-specific goals and challenges for handling streaming data, (ii) a survey and analysis of the state of the art in streaming data visualization research with a focus on how visualization design meets challenges specific to change perception and (iii) reflections on the design trade-offs, and an outline of potential research directions for addressing the gaps in the state of the art.

The State of the Art in Vortex Extraction

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Abstract: Vortices are commonly understood as rotating motions in fluid flows. The analysis of vortices plays an important role in numerous scientific applications, such as in engineering, meteorology, oceanology, medicine and many more. The successful analysis consists of three steps: vortex definition, extraction and visualization. All three have a long history, and the early themes and topics from the 1970s survived to this day, namely, the identification of vortex cores, their extent and the choice of suitable reference frames. This paper provides an overview over the advances that have been made in the last 40 years. We provide sufficient background on differential vector field calculus, extraction techniques like critical point search and the parallel vectors operator, and we introduce the notion of reference frame invariance. We explain the most important region-based and line-based methods, integration-based and geometry-based approaches, recent objective techniques, the selection of reference frames by means of flow decompositions, as well as a recent local optimization-based technique. We point out relationships between the various approaches, classify the literature and identify open problems and challenges for future work.

Data Reduction Techniques for Simulation, Visualization and Data Analysis

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Abstract: Data reduction is increasingly being applied to scientific data for numerical simulations, scientific visualizations and data analyses. It is most often used to lower I/O and storage costs, and sometimes to lower in-memory data size as well. With this paper, we consider five categories of data reduction techniques based on their information loss: (1) truly lossless, (2) near lossless, (3) lossy, (4) mesh reduction and (5) derived representations. We then survey available techniques in each of these categories, summarize their properties from a practical point of view and discuss relative merits within a category. We believe, in total, this work will enable simulation scientists and visualization/data analysis scientists to decide which data reduction techniques will be most helpful for their needs.

Generation and Visual Exploration of Medical Flow Data: Survey, Research Trends, and Future Challenges

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Abstract: Simulations and measurements of blood and air flow inside the human circulatory and respiratory system play an increasingly important role in personalized medicine for prevention, diagnosis, and treatment of diseases. This survey focuses on three main application areas. (1) Computational Fluid Dynamics (CFD) simulations of blood flow in cerebral aneurysms assist in predicting the outcome of this pathologic process and of therapeutic interventions. (2) CFD simulations of nasal airflow allow for investigating the effects of obstructions and deformities and provide therapy decision support. (3) 4D Phase-Contrast (4D PC) Magnetic Resonance Imaging (MRI) of aortic hemodynamics supports the diagnosis of various vascular and valve pathologies as well as their treatment. An investigation of the complex and often dynamic simulation and measurement data requires the coupling of sophisticated visualization, interaction, and data analysis techniques. In this paper, we survey the large body of work that has been conducted within this realm. We extend previous surveys by incorporating nasal airflow, addressing the joint investigation of blood flow and vessel wall properties, and providing a more fine-granular taxonomy of the existing techniques. From the survey, we extract major research trends and identify open problems and future challenges. The survey is intended for researchers interested in medical flow but also more general, in the combined visualization of physiology and anatomy, the extraction of features from flow field data and feature-based visualization, the visual comparison of different simulation results, and the interactive visual analysis of the flow field and derived characteristics.