Interactive Visual Analysis of Scientific Data

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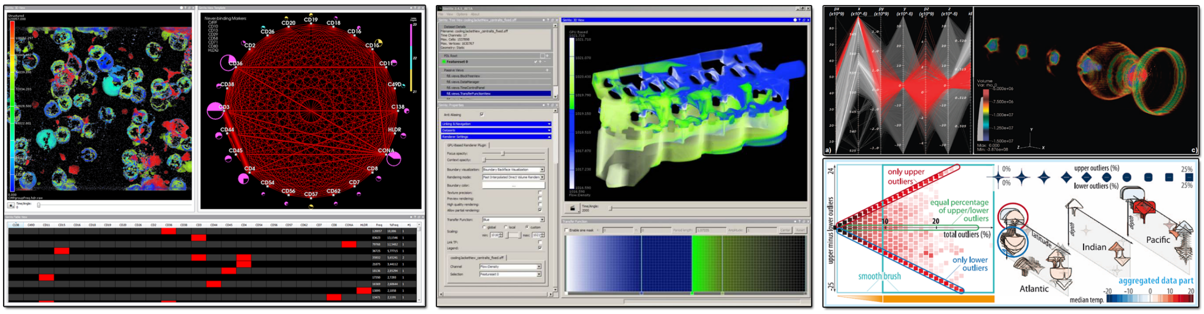

In a growing number of application areas, a subject or phenomenon is investigated by means of multiple datasets being acquired over time (spatiotemporal), comprising several attributes per data point (multi-variate), stemming from different data sources (multi-modal) or multiple simulation runs (multi-run/ensemble) [KH12]. Interactive visual analysis (IVA) comprises concepts and techniques for a user-guided knowledge discovery in such complex data. Through a tight feedback loop of computation, visualization and user interaction, it provides new insight into the data and serves as a vehicle for hypotheses generation or validation. It is often implemented via a multiple coordinated view framework where each view is equipped with interactive drill-down operations for focusing on data features. Two classes of views are integrated: *physical views* show information in the context of the spatiotemporal observation space while *attribute views* show relationships between multiple data attributes. The user may drill-down the data by selecting interesting regions of the observation space or attribute ranges leading to a consistent highlighting of this selection in all other views (*brushing-and-linking*). Three patterns of explorative/analytical procedures may be accomplished by doing so. In a *feature localization*, the user searches for places in the 3D/4D observation space where certain attribute values are present. In a *multi-variate analysis*, relations between data attributes are investigated, e.g., by searching for correlations. In a *local investigation*, the user inspects the values of selected attributes with respect to certain spatiotemporal subsets of the observation space. In this tutorial, we discuss examples for successful applications of IVA to scientific data from various fields: automotive engineering, climate research, biology, and medicine. We base our discussions on a theoretical foundation of IVA which helps the tutorial attendees in transferring the subject matter to their own data and application area. This universally applicable knowledge is complemented in a tutorial part on IVA of very large data which accounts for the tera- and petabytes being generated by simulations and experiments in many areas of science, e.g., physics, astronomy, and climate research. The tutorial also provides an overview of off-the-shelf IVA solutions. It is concluded by a summary of the gained knowledge and a discussion of open problems in IVA of scientific data.

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Tutorial Title

Interactive Visual Analysis of Scientific Data

Tutorial Length

Half-day tutorial

Why is it worthwhile?

A review of all IEEE VisWeek submissions from 2010 and 2011 showed that many of them describe software or approaches which combine several views on the investigated data. In various cases, in particular for VAST and BioVis submissions, these views are also linked and equipped with brushing facilities. From application papers it becomes obvious that different datasets showing the same subject or phenomenon need to be concurrently processed. In addition, three workshops dedicated to visual analysis were held during the past two years at VisWeek ("Visual Analytics in Healthcare: Understanding the Physicians Perspective" and "Extreme Scale Visual Analytics"). All of them received a good attendance. Altogether, this indicates a growing demand for interactive visual analysis (IVA) in the community and motivates our tutorial.

The tutorial encompasses a theoretical foundation of IVA which supports the tutorial attendees in transferring the subject matter to their own data and application area and helps them in engineering their own IVA solutions. This foundation is complemented in a tutorial part on IVA of very large data which accounts for the tera- and petabytes being generated by simulations and experiments in many areas of science. Based on the theoretical part, successful applications of IVA to scientific data from various fields are discussed: automotive engineering, climate research, biology, and medicine. These discussions go beyond the direct application of techniques that were introduced in the theoretical part. They also cover new techniques, e.g., from statistics and knowledge discovery (printed in bold in the tutorial syllabus section), which proved to be particularly useful for a specific application. Hence, the tutorial attendees will continuously broaden their theoretical IVA knowledge.

The tutorial also provides an overview of off-the-shelf IVA solutions which may be particularly interesting for visualization practitioners. Each topic is presented by a leading researcher with excellent communication skills, and considerable experience in giving lectures or talks. The talks will be stimulating by also discussing open problems. All tutorial speakers, as well as their topics, do not only aim at pure academic progress but instead at contributing to solving real application problems. Their experiences and lessons-learned in interdisciplinary collaborations are included. One of the speakers will contribute his business point of view on selling IVA solutions to customers. The entire tutorial material will be made available to the attendees on a website.

Tutorial Speakers

- Steffen Oeltze, Otto-von-Guericke University of Magdeburg, Germany
- Helmut Doleisch, SimVis GmbH, Vienna, Austria
- Helwig Hauser, University of Bergen, Norway
- Gunther Weber, Lawrence Berkeley National Laboratory and University of California, Davis, US

Tutorial History

The tutorial has not been held before but has been newly designed for VisWeek 2012.

Level of Difficulty and Prerequisites

Intermediate/Advanced. We assume a basic understanding of visualization techniques in physical (e.g., surface and volume rendering, rendering modalities, glyphs) and attribute (e.g., histograms, scatter plots, parallel coordinates) space.

Intended Audience

Potential attendees are researchers interested in visualization and visual analytics who consider adopting the interactive visual analysis (IVA) methodology and engineer an according solution. Also visualization practitioners who are interested in off-the-shelf IVA solutions are addressed by the tutorial. In general, scientists who are aiming at hypotheses generation or validation based on complex spatiotemporal, multi-variate, multi-modal or multi-run data represent the target audience.

Tutorial Syllabus

The tutorial is designed as a textbook-like presentation. Besides the presentation of interactive visual analysis (IVA) solutions in different application fields, it also includes a theoretic introduction to IVA and a wrap-up comprising the lessons learned as well as open IVA problems. The proposed tutorial schedule is as follows:

I Introduction, *Oeltze* (10 min)
II Basics of Interactive Visual Analysis, *Hauser* (20 min)
III Interactive Visual Analysis of Engineering Data, *Doleisch* (25 min)
IV Interactive Visual Analysis of Biological Data, *Weber* (25 min)
V Interactive Visual Analysis of Medical Data, *Oeltze* (20 min)
— Break
VI Interactive Visual Analysis of Climate Data, *Hauser* (25 min)
VII Interactive Visual Analysis of Very Large Data, *Weber* (20 min)
VIII Interactive Visual Analysis Tools, *Weber, Doleisch, Oeltze* (45min)
IX Lessons Learned and Open Problems, *Oeltze* (10 min)

II This part constitutes the backbone of the tutorial. It equips the attendees with the theoretical background of IVA. The subject matter supports them in engineering their own IVA solutions and also in following the subsequent application part of the tutorial. Basic IVA concepts such as physical views, attribute views, features, and brushing-and-linking are introduced. Further, the three patterns of explorative/analytical procedures in IVA are explained: feature localization, local investigation, and multi-variate analysis. Extensions of the basic IVA concepts are also discussed, for instance, *smooth brushing*, which facilitates the definition of a gradual course between "interesting data" and "data not of interest" [DH02]. This smooth *degree of interest* facilitates the use of generalized focus plus context (F+C) methods which reduce cluttering in resulting visualizations and draw a user's attention to the most important details. The theoretical part of the tutorial has evolved over years in university lectures and was continuously fine-tuned and updated.

III In the automotive engineering industry, computation fluid dynamics (CFD) simulations are employed in developing and testing new products. These simulations result in large amounts of time-dependent, multi-dimensional, multi-variate data. The analysis of such data is challenging, but also important to speed up simulation-cycles, which leads to shortening design and development cycles. In this tutorial part, we present an IVA framework and demonstrate how engineers benefit from using it during their routine analysis, as well as for exploring new phenomena [DH12]. We apply the framework in three case studies from automotive engineering. Within the first study, the effectiveness of a diesel particular filter being part of a diesel exhaust system for passenger cars is investigated [DMG*04]. We show that the IVA framework is especially useful here since multiple data attributes must be considered in order to answer a specific application question. Within the second case study, the combustion inside a specific diesel engine is examined [DMG*05]. This requires an extension of the framework to time-varying grids. The visual analysis and exploration of fluid flow in a cooling jacket represents the third case study [LGD*05].

Here, we focus on combining IVA, **automatic feature extraction methods** and state-of-the-art flow visualization techniques.

IV During animal development, complex patterns of gene expression provide positional information within the embryo. To better understand the underlying gene regulatory networks, the Berkeley Drosophila Transcription Network Project (BDTNP) has developed methods that support quantitative computational analysis of three-dimensional (3D) gene expression in early Drosophila embryos at cellular resolution. Two aspects of gene expression are of particular interest: (i) gene expression patterns defined by the spatial locations of cells expressing a gene, and (ii) relationships between the expression levels of multiple genes. For IVA it is useful to provide two corresponding classes of data views: (i) physical views based on the spatial relationships of cells in the embryo, and (ii) attribute views which plot expression levels of multiple genes with respect to each other [WRH*09]. Integrating user-guided **data clustering methods** into this system aids in the exploration of these new complex datasets [RWH*10]. IVA is also useful in the analysis of ChIP-chip in vivo DNA binding. Most analyses have focused on qualitative descriptions of whether genomic regions are bound or not. There is increasing evidence, however, that factors bind in a highly overlapping manner to the same genomic regions and that it is quantitative differences in occupancy on these commonly bound regions that are the critical determinants of the different biological specificity of factors. As a result, it is critical to have a tool to facilitate the quantitative visualization of differences between transcription factors and the genomic regions they bind to understand each factor's unique roles in the network [HWL*10].

V In medicine, the generation and diagnostic evaluation of multi-field and multi-modal data are gaining importance. Instead of a single 3D dataset, several datasets are acquired at different points in time and with different imaging modalities. Furthermore, additional data may be derived from the measured data. The complexity of the data requires visual analysis approaches that guide the user to interesting portions of the data by incorporating his/her a priori knowledge and by providing interactive filtering mechanisms. In this tutorial part, we present an interactive visual analysis approach [ODH*07], which comprises, among others, a **data dimension reduction** step (Principal Component Analysis) and a **data clustering and classification** step. The approach has been applied to perfusion data in breast cancer diagnosis [GPTP10] and in the diagnosis of ischemic stroke [OHR*09] and Coronary Heart Disease [ODH*07]. Perfusion data represent a special instance of medical multi-field data. After the injection of a contrast agent (CA), several volumes covering the object of interest are acquired over time during a single imaging scan and additional parameters are derived from the data which characterize the temporal course of the CA accumulation.

VI In climate research, massive amounts of data are generated by means of climate observations and model-based simulations. The generated data is often time-dependent, multi-dimensional and multi-variate. IVA concepts are employed in exploring the data and in generating new hypotheses for subsequent statistical validation [KLM*08]. One of the most prominent topics in climate research is the investigation, detection, and allocation of climate change. In this tutorial part, we demonstrate how IVA helps identifying climate parameters and regions in the atmosphere (e.g., certain height layers) which can act as sensitive and robust indicators for climate change [LSL*09]. We further show that integrating and brushing **statistical moments** (mean, variance, skewness, kurtosis) in an IVA framework helps the climate researcher in detecting data trends and outliers [KFH10]. Climate data may consists of different parts given on different spatial grids over time, e.g., an atmosphere and an ocean part from a coupled climate model. We discuss an interface for IVA of such heterogeneous scientific data [KMDH11]. The interface establishes a correspondence between grid cells, it defines how features specifications are transferred between different parts and it integrates an update mechanism which keeps the feature specification in both data parts consistent during the analysis.

VII A central challenge in modern science is the need to quickly derive knowledge and understanding from large, complex collections of data. To apply interactive visualization analysis effectively to datasets where a single time step can exceed storage sizes of 200GB, it becomes necessary to combine visualization with high-performance scientific **data management techniques**. For example, using state-of-the-art index/query technology, it becomes possible to identify efficiently particles selected by a brush and create histogram-based parallel coordinate plots of large datasets. This approach, while originally applied to accelerator science, is generally applicable to a broad set of science applications, and is implemented in a production-quality visual data analysis infrastructure [RPW*08]. Using the same technology it is possible to perform "cumulative" queries that work on both an intra- and intertime step basis. The results of such queries are visualized as frequency histograms and are the input for secondary queries, the results of which are then visualized [SWR*12].

VIII In this part, an overview of off-the-shelf IVA solutions will be given and three solutions will be presented in detail: `ParaView` †, `VisIt` ‡, and `SimVis` §. They have been chosen since they incorporate not only attribute but also physical 2D/3D views which are crucial in depicting spatial relations. The open-source software `ParaView` is built on top of the Visualization Toolkit (VTK) and is widely used in the visualization community. It has recently been extended by basic IVA concepts such as brushing and linking. The open-source software `VisIt` provides dedicated support for interactively analyzing and visualizing extremely large data sets [CBW*11] and exploits IVA concepts in this context [BJA*09]. As a professional, commercial IVA solution `SimVis` will be presented. `SimVis` is used by various customers working in many different scientific and industrial areas. It has also been employed in several research publications, among which 7 IEEE TVCG papers are listed.

† www.paraview.org, Kitware, Clifton Park, NY, U.S.

‡ wci.llnl.gov/codes/visit, Lawrence Livermore National Laboratory, Livermore, CA, U.S. and DOE SciDAC Institute of Scalable Data Management, Analysis and Visualization

§ www.simvis.at, SimVis GmbH, Vienna, Austria

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Steffen Oeltze is a postdoctoral fellow at the Computer Science Department at the Otto-von-Guericke University of Magdeburg (UoM). His research interests are in medical visualization, in particular the visualization of vasculature and the visual analysis of 4D-perfusion and blood flow data, and in biological data visualization, for instance the visual analysis of protein colocalization studies. In 2004 and 2008 he received the "Karl-Heinz-Höhne" award (2nd and 1st place) for his scientific work on the visualization of vasculature with convolution surfaces and the interactive visual analysis of perfusion data, respectively. He won the 2005 and 2008 annual research awards of the computer science faculty at the UoM for his work on vessel visualization, published in IEEE Transactions on Medical Imaging, and his scientific overall achievement, respectively. Steffen organized the tutorials "Visual Medicine: Techniques, Applications and Software" and "Advanced Visual Medicine: Techniques, Applications and Software" at IEEE Vis in 2006 and in 2007. He was a speaker at the tutorial "Advanced Visual Medicine: Techniques for Visual Exploration & Analysis" at IEEE Vis in 2008. Steffen received the diploma (M.Sc.) degree in computational visualistics from the UoM in 2004. In 2010, he received his Ph.D. in computer science from the UoM.

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Helmut Doleisch received the graduate degree in computer science in 1999 from Vienna University of Technology, Austria, where he worked for two years as an university assistant at the Institute of Computer Graphics. He joined the VRVis Research Center, Vienna, Austria, in late 2000. There he researched the basic SimVis-Technology while working on his PhD. After receiving the PhD degree in 2004, he headed the "Visual Interactive Analysis" Group at the VRVis Research Center as a key researcher, supervising students and leading multiple application-oriented research projects in the scope of interactive visual analysis of large and complex simulation data. In 2008, he founded the spin-off company SimVis GmbH (www.simvis.at), where he holds the position of the CEO since then. His research interests are in the areas of interactive visual analysis, flow visualization, and multi-variate data visualization, and more specifically, in the visualization of large amounts of simulation results. He co-authored over 30 papers, most of them on interactive visual analysis of simulation data. He received several best paper awards and won the IEEE Visualization Contest 2004 on "Interactive Visual Analysis of Simulated Hurricane Isabel". He is a member of IEEE, VDI, NAFEMS, and EGU.

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Helwig Hauser graduated in 1995 from Vienna University of Technology (TU Wien), Austria. In 1998, he finished his PhD project on the visualization of dynamical systems. In 2003, he finished his Habilitation at TU Wien entitled "Generalizing Focus+Context Visualization" and in 2006 this work was awarded with the Heinz-Zemanek Preis. Helwig Hauser is member of the EuroVis Steering Committee, the TopoInVis Steering Committee, and has served / is serving on the Editorial Boards of Computers & Graphics, Computer Graphics Forum, and IEEE Transactions on Visualization and Computer Graphics. He also (co-)chaired several events, including TopoInVis 2011, EuroVis 2011, and PacificVis 2012, more recently. After first working for TU Wien as assistant (since 1994) and later as assistant professor, he changed to the new VRVis Research Center in 2000. There, he led the basic research group on interactive visualization (until 2003) before he became the scientific director of VRVis. Since 2007, he is a full professor in visualization at the University of Bergen in Norway. Helwig Hauser is promoting interactive visual analysis for about twelve years (with dozens of publications and a larger number of talks, also including several invited/keynote talks).

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