Visualization and Visual Analysis of Multi-faceted Scientific Data: a Survey

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Abstract—Visualization and visual analysis play important roles in exploring, analyzing and presenting scientific data. In many disciplines, data and model scenarios are becoming *multi-faceted*: data are often spatio-temporal and multi-variate; they stem from different data sources (multi-modal data), from multiple simulation runs (multi-run/ensemble data), or from multi-physics simulations of interacting phenomena (multi-model data resulting from coupled simulation models). Also, data can be of different dimensionality or structured on various types of grids that need to be related or fused in the visualization. This heterogeneity of data characteristics presents new opportunities as well as technical challenges for visualization research. Visualization and interaction techniques are thus often combined with computational analysis. In this survey, we study existing methods for visualization and interactive visual analysis of multi-faceted scientific data. Based on a thorough literature review, a categorization of approaches is proposed. We cover a wide range of fields and discuss to which degree the different challenges are matched with existing solutions for visualization and visual analysis. This leads to conclusions with respect to promising research directions, for instance, to pursue new solutions for multi-run and multi-model data as well as techniques that support a multitude of facets.

Index Terms—Visualization, interactive visual analysis, multi-run, multi-model, multi-modal, multi-variate, spatio-temporal data.

1 INTRODUCTION

OUR society is confronted with rapidly growing amounts of scientific data that arise in various areas of science, engineering, and others. Examples are multi-variate and time-dependent climate simulations, computational fluid dynamics, sensor logs, and medical scans. Visualization has proven to be very useful to explore, analyze and gain insight into such data [1]. However, due to the increasing complexity and heterogeneity of scientific data, new sophisticated approaches are needed [2]. Interactive visual analysis is a still new multi-disciplinary field that combines analytical and interactive visual methods [3], [4], [5], [6]. Interaction schemes such as linking and brushing enable a powerful drill-down mechanism into the represented information [7].

1.1 Multi-faceted Scientific Data

The integration of abstract data from multiple sources is more common in *information visualization* (InfoVis), for example, when visualizing relational databases [8], [9] or web data [10]. In this survey, however, we focus on challenges that arise from the heterogeneous nature of *scientific data*. Such data are usually given with a strong inherent reference to space and often also time and result from a scientific data acquisition method such as

simulation or imaging. When talking about *multi-faceted* scientific data, we consider mainly the following facets: (f1) *spatio-temporal* data that represent spatial structures and/or dynamic processes; (f2) *multi-variate* data consisting of different attributes such as temperature or pressure; (f3) *multi-modal* data stemming from different acquisition modalities (data sources); (f4) *multi-run* data (also called ensemble data) stemming from multiple simulation runs that are computed with varied parameter settings; and (f5) *multi-model* data resulting from coupled simulation models that represent physically interacting phenomena [11] or neighboring climate compartments such as ocean and atmosphere [12]. Current methods for visualization and visual analysis typically address only one data facet (see Fig. 1). In practice, however, we increasingly often find model and data scenarios that are more heterogeneous. A central goal is "to synthesize different types of information from different sources into a unified data representation" [4].

Before going into more details with respect to our survey, examples of different facets of scientific data are discussed together with related challenges for visualization research. Advanced computing allows the simulation of dynamic phenomena on high-resolution grids over large timescales (e.g., global climate models or automotive engine simulations). The visualization and analysis of such spatio-temporal data (f1) is challenging and a lot of research has been dedicated to this facet. A number of surveys give a good overview [13], [14], [15], [16], [17], [18]. Analysts commonly investigate how their data relate to time and space. They want to study changes, compare different points in space and time, and uncover spatio-temporal patterns (e.g., special events or repeated behavior). A frequent goal is to integrate data from multiple time steps in a single image, for instance, by using a linear or cyclic axis to represent time [17],

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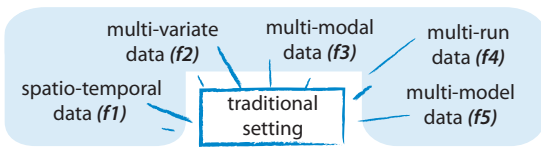
Fig. 1. Multiple facets of heterogeneous scientific data.

Fig. 2. Fluid–structure simulation of warm water flow though a cooler aluminum foam [37]: The fluid and solid part of the simulation are connected by an interface that relates grid cells sharing a common face and allows the exchange of properties such as heat.

[18]. Alternatively, different locations or time steps can be shown side-by-side to facilitate comparison [19], [20]. The decision whether to use a 2D or 3D representation is a general question in visualization and usually depends on the task at hand [7], [13], [18]. However, some kinds of data such as volumetric or 3D flow data inherently suggest a 3D representation. Automated analysis methods are often applied in order to *abstract* time-related data characteristics, for example, by computing temporal data trends [21] or statistical aggregates such as mean values or standard deviations [15].

Scientific data often contain multiple attributes per space-time location. The interactive visualization of such multi-variate data (f2) is challenging too [2]. Wong and Bergeron [22] and, more recently, Fuchs and Hauser [23] give comprehensive overviews on the topic. Interesting data subsets (*features*) can often be extracted only when considering multiple data attributes and their relations. Many visual analysis approaches, therefore, integrate computational methods such as statistics or dimensionality reduction [24], [25]. When *fusing* (intermixing) multiple scalar fields in a visualization, one typically has to cope with cluttering and occlusion. Multi-variate data are often analyzed using multiple linked views that support interactive feature specification via brushing [26].

While multi-variate data usually result from one data modality and describe different physical (or other) properties for the same spatio-temporal locations, multi-modal data (f3) stem from multiple data sources. Examples are different medical scans such as computer tomography (CT) or magnetic resonance imaging (MRI), which have to be co-registered first [27], [28]. Another example are data from different numerical models that simulate the same physical object or phenomenon (e.g., different atmospheric or ocean models). Such data can be given on various data grids (e.g., 2D/3D, unstructured or hybrid) with different temporal or spatial resolutions. Accordingly, one challenge is to fuse such multi-modal data in the visualization [23], [29]. An analytic task can be, for instance, to compare data from a climate simulation with observational measurements in order to find errors and to reduce uncertainties [30].

In areas such as climate research [12], [31] and engineering [32], multi-run simulations (f4) are increasingly often performed to study the variability of a simulation model and to understand the model sensitivity to certain control parameters. The simulation is repeated multiple times with varied parameter settings (also called an ensemble simulation). In the resulting data, a collection of values co-exists for the same data attribute at each space-time location [33] (one value for each simulation run). The goals of such a *sensitivity analysis* include [34]:
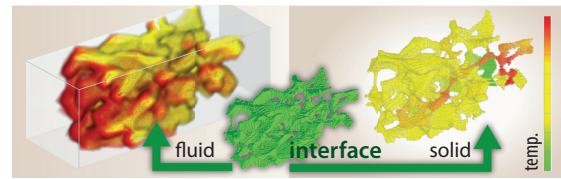
the identification of model parameters that require additional research, which also reduces the output uncertainty; identifying control parameters that are strongly correlated with the simulation output; or finding insignificant parameters that can be eliminated from the model [34]. In the analysis, the data is often aggregated, for example, by computing statistical properties with respect to all runs [31], [35]. While often only the summarized information is analyzed further, it can be useful to integrate and related both multi-run and aggregated data in the visual analysis [36], [37]. It is generally very challenging to depict and analyze a larger number of co-located data volumes; to extract interesting patterns and trends that occur in different runs; to investigate how many of the runs exhibit a certain pattern; or to study correlations between input and output variables of the simulation (compare also to Wilson and Potter [38]).

While dynamic flow is traditionally simulated with respect to a rigid (or open-ended) boundary, fluid and solid parts interact during modern *multi-physics* simulations [11]. The solid part, for instance, can be heated or deformed by the surrounding flow. The different data parts are commonly modeled individually on spatially adjoining grids that are connected by a so-called interface (see Fig. 2). During the simulation, the parts can interact with each other via the interface and exchange physical properties such as heat. In the climate system, as another example, components such as atmosphere, ocean, ice, and land interact with each other, as well. Atmosphere and ocean, for instance, exchange through thermal absorption, precipitation and evaporation [12]. To understand such dynamics, models for the different climate components are coupled in the simulation, commonly with additional coupler modules. Creating a coherent visualization from such multi-model scenarios (f5) with two or more interacting data parts (e.g., fluid and structure or atmosphere and ocean) is a challenge for visualization, which has been hardly addressed so far [37]. How can, for instance, feedback and relations between spatially neighboring data parts be investigated?

We focus on the data facets described above, since they are typical examples for scientific visualization. There exist also other interesting modalities such as pictures, video or text. Textual information, for example, can provide semantic context to the data and will become more important in the future, also in scientific visualization (e.g., patient reports or description of genes). A detailed description of these types, however, is beyond the scope of this survey.

1.2 Survey Structure and Contributions

In this survey, we give an encompassing view on the visualization and visual analysis of multi-faceted scientific data. We explain our choice of which facets to focus on and which to only survey in terms of an overview. Based on an extensive literature review, we have identified a number of techniques that are common to all the facets of scientific data. We propose a novel categorization of approaches based on characteristics of these techniques and discuss them with respect to the different facets. We identify mature areas in visualization and visual analysis as well as promising directions for future research.

The visualization of spatio-temporal (f1) and multi-variate (f2) data, for instance, have been broadly investigated, and a lot of good solutions are available. Although these areas belong to the topics discussed here, we only touch them briefly and refer to other good overview articles. As part of our contribution, we add a discussion of newer approaches that came up more recently. The primary focus of this survey, however, is on multi-modal (f3), multi-run (f4) and multi-model (f5) data. Especially multi-run and multi-model data scenarios are relatively new to the visualization community [33], [37], even though these types of data are getting more popular in important application domains such as engineering, climate or multi-physics research. While we aim at putting existing approaches for multi-faceted scientific data into a broad common framework, not all related work can be discussed in such an article. We consider it valuable, however, to present an integration of such a broad spectrum of topics in a joint survey.

The remainder of this paper is organized as follows: before going into detail with respect to related work, some basic notations are clarified in section 2. We also present our classification of approaches. Section 3 discusses important concepts in interactive visual analysis such as coordinated multiple views and the combination of computational analysis and interactive visualization. Section 4 addresses the visualization and visual analysis of spatio-temporal data (f1), and section 5 does this for multi-variate scientific data (f2). The representation, fusion and comparison of multi-modal data (f3) are described in section 6. Section 7 discusses the visual analysis of multi-run data (f4), and section 8 addresses challenges for multi-model data (f5). Finally, an outlook to promising future research and open challenges is given in section 9. In sections 4 to 7, we distinguish between approaches for representation (in terms of visual metaphors), computational analysis and interaction, which also integrate analytical/exploratory procedures.

2 TERMINOLOGY AND CATEGORIZATION

In this section, some basic notations are clarified first. Next, we propose our categorization of approaches for multi-faceted scientific data with respect to common visualization, analysis and interaction methods.

A continuous data model is very often assumed with *scientific data*, which means that the data can be interpolated between discretely sampled values [39]. In many cases, such data can be denoted as $f_i(\mathbf{x})$ where different data values f_i (e.g., velocity vectors, temperature or pressure values) are measured or simulated with respect to points $\mathbf{x}$ in an n-dimensional domain. The domain (i.e., the independent data dimensions) can be 2D or 3D space, time, but also independent input parameters to a simulation model. *Multi-run* data (f4), for example, stem from a simulation that is repeated multiple times with varied parameter settings, leading to a larger number of co-located data volumes given for the same space-time [12], [33], [38]. In this understanding, the word *multi-dimensional* (f1) refers to the dimensionality of the independent variables, while *multi-variate* (f2) refers to the multitude of dependent variables [22].

Categorization of approaches: Based on a literature review of more than 200 papers that address at least one facet of modern scientific data, we aim at identifying common groups of visualization, analysis and interaction methods. The different categories are described in the following and represented in the columns of Table 1. Similar to the categorization of Bertini and Lalanne [24], the groups cover a broad spectrum, ranging from techniques that mainly address *visual mappings*, i.e., how to represent the data (left in Table 1), to methods that focus on *computational analysis*, i.e., what are the main characteristics or features of the data (right). Additionally, many approaches rely on *interaction* concepts such as linking and brushing, zooming, panning, or view reconfiguration [40]. Although often discussed separately, visualization, interaction and computational analysis clearly are not mutually exclusive. The tight integration of all three levels is a major goal in visual analysis (see Sec. 3).

Approaches for *visual data fusion* aim at intermixing different facets of scientific data in a single visualization, using a common frame of reference. Different time steps can, for instance, be shown along a spatial axis (e.g., as function graphs or on a spiral). According to Fuchs and Hauser [23], multi-variate data can be fused at different stages of the visualization pipeline, for instance, when mapping variables to different visual properties (e.g., glyphs, texture or color), during rendering, or in image stage using layering techniques. For multi-modal data, the different data sources first need to be registered and normalized to each other in order to make them comparable (e.g., resampling to a common grid). The visualization thereby has to be designed carefully to avoid the introduction of artifacts that can be erroneously interpreted as features [29]. Multi-run data can, for example, be represented as families of data surfaces [41] or spaghetti plots [42]. However, it is often not practical to directly visualize such data since they can consist of multiple co-located volumes of spatio-temporal (and often multi-variate) data. Consequently, some approaches compute summary statistics from the multiple runs, which are represent by glyphs or box plots [33], [37], [43].

Comparative visualization investigates the data for similarities and differences [30]. Examples are the comparison of different time steps, spatial locations, data variables or modalities. Dependent on the level of data

TABLE 1
Categorization of techniques for the visualization and visual analysis of multi-faceted scientific data.

	visual mapping	interactive visual analysis				computational analysis
	visual data fusion	*relation & comparison*	*navigation*	*focus+context & overview+detail*	*interactive feature specification*	*data abstraction & aggregation*
multi-dimensional	maps [13], [14], [92]; Helix glyphs [93]; flow maps [105]; function graphs [70], [71], [72]; Time Histograms [94], [110], [111]; chrono volumes [98]; illustrative techniques [99]; texture-based flow vis. [100]	2-tone coloring [20]; Helix glyphs [93]; juxtaposed views [19], [110]; difference views [107]	search, zooming and panning [40], [54]	2-tone coloring [20]; multi-level focus+context [71]; pixel-based multi-resolution techn. [104]	brushing [21], [70], [71], [95], [113]; transfer functions [110], [111]	aggregation [15], [103], [105]; trends [21]; flow features [82]; clustering [83], [84], [110]; PCA [17], [78], [85]; SOM [89], [90]; KDE [106], [107]; information theory [108]; wavelet analysis [109], [110]
multi-variate	attribute views [22], [50], [67]; color & texture [119]; layering [115], [124], [126]; 2-level volume rendering [127], [128]; glyphs [120], [121], [122], [123], [124], [125]	correlation fields [133]; operators [134]; multiple linked views [9], [26], [29], [73], [74], [76]	grand tour [47]; ScatterDice [46]; ranking & quality metrics [48], [130], [131], [132]	illustrative vis. [115], [116]; oulier-preserving methods [69]; smooth brushing [80]	brushing [9], [50], [74], [75], [112]; multi-dim. transfer func. [114], [115]; machine learning [91], [135], [136]	clustering [68], [130]; data binning [69]; PCA [78]; MDS [86], [87]; SOM [88], [89]; projections [47], [48], [130], [132]; point clouds [129]
multi-modal	resampling [138]; data model [142]; illumination model [143]; multi-volume rendering [128], [139], [143], [144], [145], [146]	difference views [107]; multi-image view [153]; nested surfaces [31], [154], [156]; features [44], [155]	viewpoint selection [49]	cutaway views [147], [139], [49]	transfer functions [143], [144]	registration [27]; mutual information [28]; comparison metrics [148], [151], [152], [133]
multi-run	glyphs & box plots [37], [43], [162], [163], [164]; shape descriptors [164]; families of surfaces [41]; spaghetti plots [35], [42], [165]	aggregated & multi-run data [36], [37], [41], [174]; HyperMoVal [51], [52]	aggregated & multi-run data [36], [37], [41]; parameter space nav. [51], [52]	aggregated & multi-run data [36], [37], [41]; simulation process vis. [173], [174]	trends & outliers [36], [37], [41]; visual steering [172]	overview statistics [31], [35], [36]; projections [41], [51], [170], [171]; operators [33]; PCA [169]; clustering [167], [168], [169]
multi-model	feature fusion across multiple data parts [37]	feature relation across data parts [37]	x	x	feature spec. across data parts [37]	x

abstraction, scientific data can be compared at the image, data or feature level [44]. In the context of information visualization, Gleicher et al. [45] classify comparative visualization according to three categories: 1) juxtaposition, which compares objects side-by-side; alternatively, 2) the data can be overlaid in the same frame of reference (similar to visual fusion [29]); or 3) computed relationships can be explicitly encoded, for example, by showing differences or correlations. Additional interaction techniques such as linking and brushing or repositioning of objects can facilitate visual comparison [45].

Navigation is an important task in visualization and can be done manually [40], [46], automatically [47], or computationally assisted [48], [49]. The user typically explores the data by zooming, rotating or panning. Selecting a good viewpoint is a challenge for volumetric data [49]. In the context of multi-variate data, it is very challenging to find those attributes that describe important data characteristics such as correlations or outliers. Using an overview visualization such as a scatterplot matrix [46], [50], the user can select an interesting attribute combination. Alternatively, views can be ranked by computing quality measures [48]. Navigating the space of input and output variables of a multi-run simulation is highly challenging as well [51], [52].

Focus+context visualization can be generalized as the "uneven use of graphics resources (space, opacity, color, etc.)," where the focus is shown in detail and the context is provided for orientation or navigation purpose [53]. Such methods typically rely on interaction, where the user specifies the data in focus (e.g., by pointing, querying or brushing). While related visualizations aim at seamlessly integrating focus and context in a single view, *overview+detail* techniques spatially separate both con-

cepts (e.g., using juxtaposed views). Cockburn et al. [54] recently provide a survey on the related topics.

Interactive feature specification enables the user to manually select interesting data, for example, via brushing [50]. The resulting markup information can then be used to highlight and relate the selected data, for example, using coordinated multiple views (Sec. 3.1).

Closely related to manual feature specification are automated *data abstraction and aggregation*. Such analysis methods aim at algorithmically extracting meaningful values or patterns from the data, where the main data characteristics are still represented but irrelevant details are suppressed [17]. The abstracted data can then be visualized or analyzed instead of the original one. Many related approaches come from the fields of statistics, data mining, or machine learning [55]. Visual analysis aims at combining such methods with interactive visualizations, where the user can steer the analysis process (see Sec. 3).

By grouping the related work by techniques, we aim at presenting alternatives for addressing different kinds of scenarios. While we give a comprehensive view on the visual analysis and representation of multi-run and multi-model data, only selected examples for spatio-temporal and multi-variate data are discussed together with existing surveys. It should be noted that also other techniques (e.g., knowledge-assisted visualization [56] or clutter reduction) and other factors could be used for this classification, for example, visualization challenges [2], user tasks [7], [39], or application domains. Keller and Keller [57], for instance, present an early task-based categorization for visualization. They illustrate methods for a variety of data types and visualization goals. Amar and Stasko [58], more recently, discuss higher-level analytical tasks such as showing uncertainty, exposing relation-

ships, identifying cause and effect, including metadata, finding multi-variate correlations and constraints, and validating hypotheses. Some of these tasks are closely related to individual techniques discussed also here.

3 EXPLORATORY DATA ANALYSIS, VISUAL DATA MINING, AND VISUAL ANALYTICS

Visual analytics is the interdisciplinary science of analytical reasoning facilitated by interactive, visual and analytical methods [3], [4], [5], [6]. Since automated analysis methods only work reliably for well-specified problems, the idea is to combine such approaches with interactive visualization. Visualization can then, for example, support the specification of parameters at different steps of a data mining algorithm [59]. By interactively and visually exploring the original data as well as derived properties, analysts should be enabled to [4]: detect the expected and discover the unexpected; draw conclusions and generate hypotheses based on the visual information; reject or verify hypotheses; and communicate and present the results of the analytical reasoning process.

While statistical tools utilize static visualization mainly for presentation purposes (confirmatory analysis), Tukey suggests in his seminal work on *exploratory data analysis* [60] to also support direct interaction with the data. Some of the early works in InfoVis were inspired by considerations from statistics [61], [62], [63]. The analysis often follows Shneiderman's *information seeking mantra* [7]: "overview first, zoom and filter, then details-on-demand." In later work, Shneiderman [59] compares the different philosophies behind exploratory data analysis (used for hypothesis generation) and statistical hypothesis testing. The latter requires a hypothesis beforehand in order to work. Also, it is challenging to identify features that are not anticipated prior to the analysis. The author thus suggests the combination of data mining and visualization, where users should be able to express their interest in the data and specify what they are looking for (e.g., outliers or correlations).

If the data are too large and complex to be represented directly, the application of automated data abstraction techniques is often necessary. Keim proposes an according extension to the information seeking mantra for visual analytics [5]: "Analyze first, Show the Important, Zoom, filter and analyze further, Details on demand." While *visual data mining* [64], [25] mainly focuses on the integration of data mining[1] into the visualization, visual analytics [4], [5], [6] aims at integrating other methods of analytical reasoning as well (e.g., cognitive, perceptual or decision science). Excellent overviews on visual data mining are given by Keim [64], Keim et al. [25], and de Oliveira and Levkowitz [66]. Bertini and Lalanne [24] more recently survey the integration of visualization and automated analysis in knowledge discovery. Based on the degree to which such methods are combined,

the authors categorize solutions into 1) computationally enhanced visualizations, 2) visually enhanced mining, and 3) integrated visualization and mining (compare to a similar categorization by Keim et al. [25]).

In the following, typical concepts for interactive visualization and computational analysis are briefly discussed, namely coordinated multiple views (Sec. 3.1) and automated data abstraction (Sec. 3.2), respectively.

3.1 Coordinated Multiple Views

The concept of coordinated multiple views originates in the InfoVis community and has been steadily developing over the last two decades (see Roberts [26] for an overview). Different data variables are shown, explored and analyzed in multiple linked views that are utilized side-by-side. The views include histograms, scatterplot matrices [46], [50], parallel coordinates [67], [68], [69], or function graphs [70], [71], [72]. Data can be interactively selected (*brushed* [50]) in a view, the related data items are instantly highlighted in all *linked views* (compare to Polaris/Tableau [9] or the XmdvTool [73], for example). Logical combinations of brushes across multiple views support the specification of complex features, for example, in a hierarchical feature definition language [74]. In cross-filtered views [75], as another example, brushing filters between pairs of views can be enabled/disabled and the data are filtered, accordingly. Relationships between different variables can thus be explored, also across multiple datasets. Several visual analysis frameworks support the computation of new data attributes from existing ones, which facilitates the investigation of features [3], [9], [26], [74], [75].

Interaction and flexibility of the application are both crucial for visual analysis. The user should be able to query data in many different ways and quickly change what data portions are shown and how they are represented [9], [40]. ScatterDice [46] is such an example where the user explores multi-variate data using scatterplots. A scatterplot matrix [50] gives an overview of the possible axis combinations in a plot and is used for navigation. Transitions between the scatterplots are then performed using animated 3D rotations. Features can be explored and iteratively refined via brushing.

SimVis [74], WEAVE [76] and PointCloudXplore [77] are just three examples of visual analysis systems for scientific data. Such frameworks link *attribute views* such as scatterplots or parallel coordinates with *3D views* for volumetric data (usually given on grids over time). This combination enables the analyst to investigate brushed features also in the spatial context (compare to the three typical patterns of visual analysis of scientific data [78], i.e., feature localization, multi-variate analysis, and local investigation). Instead of a binary selection information, some systems integrate a fractional *degree-of-interest* attribution ($DOI_j \in [0, 1]$ for each data item j, compare to the DOI information in generalized fisheye views [79]). With *smooth brushing* [80], a transition can be specified around the main region of interest, where the DOI information gradually changes (compare also to ramped brushing in the XmdvTool [73]). The DOI values are then used in all

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1. Data mining denotes the algorithmic extraction of valuable patterns and models from data. It is part of a more general process of *knowledge discovery in databases* (KDD), which also includes steps such as data preparation, selection and cleaning [65].

linked views to visually discriminate interesting features (focus) from the rest of the data (context), leading to a *focus+context visualization* [53], [71], [74], [81].

3.2 Automated Data Abstraction

Typical (semi)automated analysis methods that are often combined with InfoVis techniques include [24], [25]: *data reduction* via sampling or algorithmic feature extraction [82]; *clustering* [68], [83], [84] where data items are grouped by similarity; and *dimensionality reduction* that aims to reduce the data dimensionality while maintaining the higher-dimensional data characteristics. Dimensionality reduction approaches include: principal component analysis [17], [78], [85] (PCA), which transforms multi-variate data into an orthogonal coordinate system that is aligned with the greatest variance in the data; multi-dimensional scaling [86], [87] (MDS), where higher-dimensional data items are mapped into a lower-dimensional space while preserving the dissimilarities between the items;[2] and self-organizing maps [88], [89], [90] (SOM) which represent an unsupervised learning method that reduces the data dimensionality and also provides a classification of the data. An issue with dimensionality reduction approaches is, however, that it can be hard to mentally relate the derived attributes to the original data. One solution can be to analyze both side-by-side in a multiple views framework with linking and brushing (see Oeltze et al. [78], for instance).

Ma [91] suggests to go a step beyond visual data mining by integrating machine learning into the analysis process. Such methods could learn from previous analysis sessions and input data, and abstract away many details of the utilized algorithms, for instance, using case-based reasoning (compare to an infrastructure supporting knowledge-assisted visualization [56]). Only high-level decisions are then left to the user by providing an "intelligent interface" for the visual analysis [91].

4 MULTI-DIMENSIONAL DATA

Multi-dimensional data such as time-varying 3D measurements and simulations are ubiquitous in disciplines such as medicine, climate research, or engineering. Being able to understand time-related developments allows one to "learn from the past to predict, plan, and build the future" [18]. When visualizing the data, time and space can be treated "just" like any other data attribute using parallel coordinates, scatterplots, or other information visualization techniques [6], [18]. In many applications, however, the independent dimensions of time and space have a semantic meaning and often play a central role in the data. Accordingly, there has been a lot of work in related fields such as cartography [92] or geovisualization [13], [14]. A number of useful reviews have been published on the visualization and analysis of spatio-temporal data [13], [14], [15], [16] as well as time-dependent data [17], [18]. According to Andrienko et al. [14], approaches for spatio-temporal data can be

categorized into the visualization of raw data, computed summaries, or automatically extracted features.

This section gives a brief overview on methods that address mainly the spatial and/or temporal characteristics of scientific data. Such data are often multi-variate as well, which is elaborated in further detail in section 5. Related surveys are discussed together with selected examples. In this context, the following subsections address the visual representation (Sec. 4.1), computational analysis (Sec. 4.2), and interactive methods (Sec. 4.3) for spatial and temporal data.

4.1 Representation of Multi-dimensional Data

Aigner et al. [18] give a systematic view on the visualization of time-oriented data. In their categorization, they consider different characteristics of the time axis such as temporal primitives (discrete points vs. time intervals) or the structure of time (linear vs. cyclic vs. branching time). These considerations are important when designing a visual analysis system, since they address the data validity and the possible relations among temporal primitives [18]. Common approaches for time-varying data include automatic animations or interactive visualizations. The latter, for instance, show the data at different time steps (e.g., juxtaposed views) or along a common time axis (e.g., function graphs or spirals). Selected visualization methods for spatio-temporal data are discussed in the following.

Time-varying data can be represented in a single view by showing them with respect to a linear or cyclic time axis [18]. The latter supports the comparison of different points in time and the analysis of recurring patterns such as seasonal trends. An example for such an approach are Helix glyphs [93] that can be placed on a geographic map (see Fig. 3c). The "tunnel view" at the bottom of the figure reveals hidden information by increasing the ribbons height and radius for each time step. The ThemeRiver [72] is an example visualization that uses a linear time axis. Thematic changes in large document collections are depicted, where the number of occurrences per topic is represented as the width of the corresponding river band (see Fig. 3a). The Time Histogram [94] is another example showing consecutive 1D histograms of the data for every time step.

Two-tone coloring [20] is an example for an integrated overview+detail technique, which enables the compact representation of many time series (details) in an overview visualization (see Fig. 3b). By showing the data values of each time series as a combination of two colors, the actual values can be read out more precisely as compared to using a continuous color map. Other approaches [70], [71], [74], [95] use color and saturation for a focus–context discrimination and are discussed in conjunction with interactive feature specification (Sec. 4.3).

Spatio-temporal data have additional characteristics, for instance, that "near things are more related than distant things" (Tobler's first law of geography [96]) or that events can happen at different spatio-temporal scales [14]. Geospatial data are often shown on cartographic maps, following a set of well-established con-

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2. Since MDS also maintains the higher-dimensional structure of the data, it is well suitable for subsequent clustering.
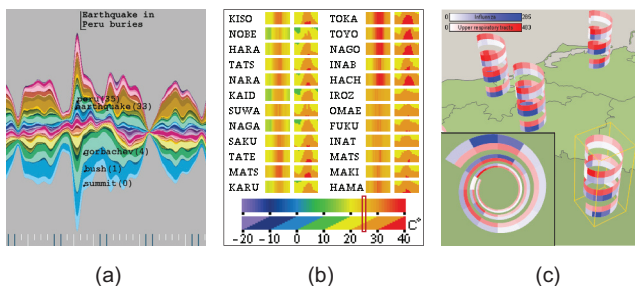
Fig. 3. Linear vs. cyclic time: (a) ThemeRiver [72] for analyzing temporal trends in document collections (image courtesy of S. L. Havre, © 2002 IEEE). (b) Visualization of temperature variations using a continuous and two-tone color map [20], respectively. The latter represents the data value of each time series as a combination of two colors (image courtesy of T. Saito, © 2005 IEEE). (c) Helix glyphs [93] for analyzing cyclic temporal patterns for two diseases (image courtesy of C. Tominski, © 2005 IEEE).
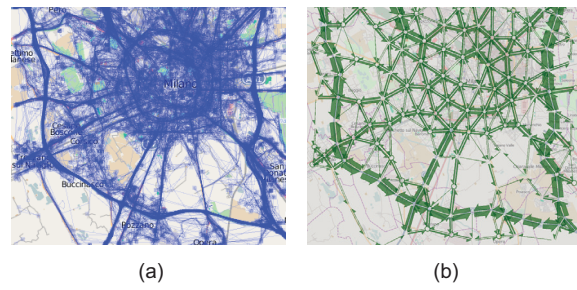

Fig. 4. Visualization of car movement data [105]: (a) Original movement trajectories are drawn using opacity. (b) Trajectories are aggregated and shown in a flow map (images courtesy of N. Andrienko, © 2010 IEEE).

ventions [13], [14], [92]. In this context, the visualization of textual information is highly relevant, for instance, by placing labels that give semantic information to the data. Many approaches for spatio-temporal data support navigation techniques such as zooming and panning [54].

Ma and Lum [16] discuss techniques that support the efficient rendering of time-dependent *volumetric data*, for example, data compression, automated feature extraction, hardware acceleration, or parallel rendering. Jankun-Kelly and Ma [97] study the (semi)automatic generation of a single or multiple transfer functions, which capture important structures in time-varying volumetric data such as regular, periodic or random pattern. The generated transfer funtion(s) can then be used for batch-mode rendering, for instance. Woodering and Shen [98] propose chronovolumes that fuse multiple time steps in a single image using color composition techniques. Joshi and Rheingans [99] present illustrative techniques that are inspired by depictions of motion in comics. Examples are speedlines, flow ribbons, or silhouettes showing the previous positions of an object.

Besides the visualization of time-dependent scalar volumes, also the visualization of time-dependent vector fields is important in many areas. Such approaches for *flow visualization* can be classified into [82], [100], [101]: 1) direct flow visualization such as color coding or arrow plots; 2) dense, texture-based approaches using, for instance, spot noise, line integral convolution, or texture advection; 3) geometric flow visualization depicting geometric objects that are extracted/computed from the flow such as streamlines, stream surfaces, streaklines, or pathlines; 4) feature-based techniques that are based on the extraction of relevant structures such as vortices or shock waves; and 5) partition-based flow visualization that subdivides the domain with respect to certain flow characteristics. While the first three categories depict basic quantities of the flow, the later two provide a more abstracted view on the data.

4.2 Analysis in Multi-dimensional Data Visualization

The approaches presented in the previous section usually reach their limits when representing larger amounts

of data with several million entries, for instance. For such data, (semi)automated data reduction and abstraction techniques need to be applied first, which transform the data into a compressed but still representative form [5]. Andrienko and Andrienko [15] give a systematic overview on the visual analysis of spatial and temporal data. Aigner et al. [17] discuss approaches for time-oriented data where visual and analytical methods are combined. Many approaches for temporal data abstraction come from the field of data mining (see Fu [102] for a recent survey). Examples include clustering, principal component analysis, or wavelet analysis.

In order to reduce the data complexity or visual cluttering, spatial and/or temporal aggregation is often applied (see López et al. [103] for an overview). With such an approach, data items sharing the same spatio-temporal domain are summarized and depicted instead of the individual data values. According to Andrienko and Andrienko [15], data aggregation can be done either by calculating data characteristics (e.g., the sum, arithmetic mean, or variance) or by grouping techniques such as clustering or binning. Aggregation techniques, however, need to be applied with care to preserve important information such as outliers [69].

Hao et al. [104] use pixel-based techniques to visualize time series data at multiple levels of aggregation, based on importance values per data interval. Andrienko and Andrienko [105] visualize movement data by combining data aggregation with flow maps. The spatial domain is subdivided into appropriate areas, based on significant points in the movement. Aggregated trajectories with common start and end points are shown with arrows (see Fig. 4b). Willems et al. [106] propose a visualization approach based on the convolution of dynamic movement data with a kernel, where the resulting density field is visualized as an illuminated height map. Daae Lampe et al. [107] propose interactive difference views based on kernel density estimates (KDEs). Quantitative differences between different categories (or bins) of aggregated data are analyzed using juxtaposed views.

Nocke et al. [83] discuss visualization techniques for clustered climate data such as the ThemeRiver [72] or Cluster Calendar View [84]. The latter approach, for instance, groups time series data over a certain period (e.g., month or day) into clusters. The clusters are then

visualized using function graphs and also encoded in color in a calendar-like representation. As a result, the frequency of occurrence of each cluster can be seen as well as the daily trends and patterns.

Dimensionality reduction techniques typically aim at reducing the data dimensionality while preserving the higher-dimensional characteristics. Aigner et al. [17] discuss the integration of PCA into the visualization of time-dependent climate data (compare also to Müller et al. [85]). Self-organizing maps [88] (SOM) can be seen as a combination of dimensionality reduction and clustering. Andrienko et al. [90] apply this approach for analyzing spatio-temporal data from two complementary perspectives: as spatial situations in different time units (space-in-time SOM) and as profiles of temporal changes at different places (time-in-space SOM). For each perspective, a SOM matrix display provides an overview of data objects arranged by similarity. The matrix is linked to views such as spatial maps, function graphs, and periodic pattern views, which enable the investigation of spatio-temporal patterns.

Concepts from *information theory* can be applied to automatically extract distinctive structures in the data. Jänicke et al. [108], for example, compute the local statistical complexity in order to identify regions with different temporal behavior than the rest of the field. The measure assesses the amount of information from the local past that is necessary to predict the local future. In later work, the same authors utilize *wavelet analysis* for exploring climate variability changes [109]. Clustering techniques based on mutual information are applied, amongst others, in order to identify coherent structures in the data. Similarly, Woodering and Shen [110] apply wavelet transformation to time-dependent volume data. The resulting multi-resolution data representation is clustered and visualized in a spreadsheet [19]. Here, multiple Time Histograms are shown that also support linking and brushing (compare to Akiba et al. [111]).

4.3 Interactive Methods for Multi-dimensional Data

While computational analysis methods typically rely on well-defined problems, certain data features are difficult to describe mathematically or hard to anticipate prior to the analysis. Consequently, many applications support interactive feature specification using brushing or querying techniques. Additionally, computational methods can be applied on-demand to facilitate the analysis.

The TimeSearcher [95] is especially designed for the visual analysis of time-dependent data using Time Boxes or angular query widgets. The latter are applied for selecting time series that have a similar slope on a sequence of time steps (compare to angular brushing for parallel coordinates [112]). Konyha et al. [70] introduce line brushes that select function graphs, which intersect a line segment drawn in the view. Akiba et al. [111] utilize a Time Histogram [94] to specify transfer functions for time-varying volume data.

Jern et al. [113] propose a coordinated multiple views system for exploring spatio-temporal multi-variate data. Cartographic maps are linked with attribute views such
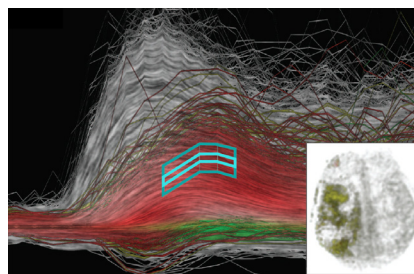

Fig. 5. Visual analysis of perfusion data acquired after an acute ischemic stroke [71]: brain tissue with reduced and delayed perfusion is selected using similarity-based brushing in the function graph view. The related tissue at risk is shown in the spatial context (inset).

as parallel coordinates that also support brushing. Interactive feature specification in multiple linked views is also an integral part of the SimVis framework [74]. Oeltze et al. [78] study the integration of both correlation analysis and PCA into the visual analysis of perfusion data. Parameters describing the temporal perfusion characteristics are extracted and analyzed together with the principal components using linking and brushing. The approach is applied in the diagnosis of breast cancer, ischemic stroke, and coronary heart disease.

Kehrer et al. [21] use brushing of derived temporal characteristics such as linear trends and signal-to-noise ratios for the steered generation of hypotheses in climate research. Spatio-temporal regions in the atmosphere are identified which can act as sensitive and robust indicators for climate change. This work is based on an extension of SimVis, which enables the interactive depiction of large amounts of time series as function graphs together with advanced brushing techniques [71]. Function graphs that are similar to a pattern sketched by the user can be interactively selected (see Fig. 5). Also, transfer functions are applied for visual clutter reduction by mapping the number of function graphs per pixel to the pixel's luminance (compare to Johansson et al. [68]). Using aggregation techniques (frequency binmaps [69]), the responsiveness of the system can be maintained, even when interacting with large amounts of time series.

5 MULTI-VARIATE SCIENTIFIC DATA

The multi-variate characteristics of scientific data are often of special interest, typically in combination with their spatial and/or temporal reference. When investigating, for instance, the fronts of a storm [114] or environmental phenomena such as the El Niño [109], multiple data attributes and their interrelation need to be considered. Johnson [2] identifies the visualization of multi-variate scientific data (also referred to as multi-field data) as one of the top challenges in scientific visualization. Comprehensive surveys on the topic are given by Wong and Bergeron [22] as well as Fuchs and Hauser [23].

In the following subsections, the representation, computational analysis, and interactive methods for multi-variate scientific data are discussed.

5.1 Representation of Multi-variate Scientific Data

Multi-variate patterns such as correlations or outliers can often be directly perceived when plotting the data in attribute space, for instance, using scatterplot matrices or parallel coordinates [22]. Such attribute views, however, are less able to convey spatial relationships of the data. Another challenge is which of the many data variables to show in order to not miss important patterns (e.g., using quality metrics [48] as discussed in Sec. 5.2). Alternative methods for spatial data such as direct volume rendering typically have difficulties encoding multi-variate charac-teristics. When fusing multiple scalar fields in a single visualization (e.g., using glyphs or layering techniques), one often has to cope with cluttering and occlusion. Different portions of the data can be represented using a set of visual styles (e.g., focus+context or illustrative visualization [53], [115], [116]). Such feature-based ap-proaches, however, typically rely on segmentation infor-mation, which can be specified, for instance, interactively via brushing or transfer functions [74], [76], [114], [115].

Multiple data values can be simultaneously repre-sented in an image using *preattentive visual stimuli* such as position, width, size, orientation, curvature, color (hue), or intensity [117], [118]. These features are rapidly processed by the low-level visual system and can thus be used for the effective visualization of large data. Special care is required, however, if several such stimuli are combined—the result may not be preattentive any more. Healey and Enns [119] propose simple texture patterns and color to visualize multi-variate spatial data. Different data attributes are encoded in the individual elements of a perceptual texture using equally distinguishable colors and texture dimensions such as element density, regularity and height. Groups of neighboring elements form texture patterns that can be analyzed visually.

Glyphs are a powerful way of encoding multi-variate data, which is often used in information visualization (e.g., star glyphs, stick figures, faces, see Ward [120] for an overview). Different data variables are represented by a glyph using a set of visual stimuli such as shape, size or color. Relations between the data variables can be directly perceived and compared, often also in the spatial context when using a hybrid visualization [23]. It should be noted that some visual cues and/or their relationships can be easier perceived than others [117], [118], [120]. An effective glyph visualization should, therefore, carefully chose and combine the utilized visual properties.

Ropinski and Preim [121] propose a perception-based glyph taxonomy for medical visualization. The authors categorize glyphs according to 1) preattentive stimuli such as glyph shape, color and placement, and 2) at-tentive visual processing, which is mainly related to the interactive exploration phase (e.g., changing the po-sition or parameter mapping of a glyph). Additional usage guidelines are proposed, for instance, that glyph shapes should be perceivable unambiguously from dif-ferent viewing directions. Kindlmann [122], for example, uses superquadric glyph shapes that fulfill this criterion. Ropinsky and Preim [121] also suggest that the mapping of data variables to glyph properties should focus the
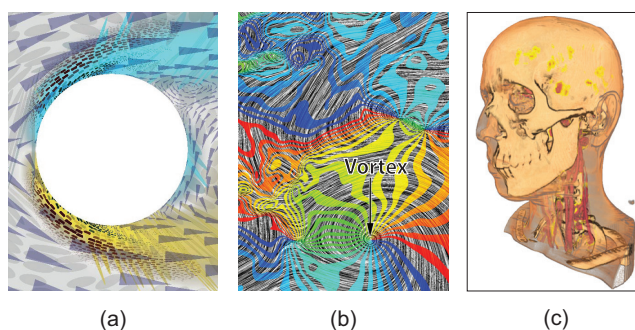

Fig. 6. Visualizing multi-variate data with layering techniques: (a) Combining glyphs, elongated ellipses, and color to show a total of nine variables [124] (image courtesy of R. M. Kirby, © 1999 IEEE). (b) Filigree graphics encoding flow direction combined with a stream-line texture [126] (image courtesy of P. C. Wong). (c) Different visual styles representing semantic information [115] (image courtesy of P. Rautek, © 2007 IEEE).

user's attention and emphasize important variables. Lie et al. [123] propose additional guidelines for glyph-based 3D visualization with respect to the different stages of the visualization pipeline. It should, for instance, be possible to perceive each visual glyph property independently (or to mentally reconstruct the depicted data values [121]). The authors discuss further design aspects of glyph-based 3D visualization such as depth perception and visual cluttering (e.g., using halos to discriminate over-lapping glyphs).

Since glyphs are typically not placed in a dense way, the space between them can encode additional informa-tion. Kirby et al. [124], for example, use concepts from painting for visualizing 2D flow. They combine differ-ent image layers with glyphs, elongated ellipses, and color (see Fig. 6a). Treinish [125] visualizes multi-variate weather data using color contouring on vertical slices and isosurfaces that represent cloud boundaries. At user-defined locations, the wind velocities are represented by a set of arrow glyphs. Additional streamlines following the wind direction are seeded at each arrow.

Multiple scalar fields can be fused in a visualization by using *2D or 3D layering*. Wong et al. [126], for example, encode different climate variables by overlaying multiple see-through layers using opacity modulation, filigree graphics, or 2D height maps. Flow features such as critical points or vortices are highlighted using enhanced color maps (see Fig. 6b). Two-level volume rendering [127], [128] considers segmentation information when visualizing 3D medical data. Different rendering tech-niques such as maximum intensity projection, direct volume rendering, or non-photorealistic techniques are combined, based on the segmentation. Viola et al. [116] propose similar focus+context techniques, which inte-grate dense as well as sparse rendering styles. Illustrative visualizations such as cut-away and ghosted views can thus be generated automatically. In later work, Rautek et al. [115] propose semantic layers for illustrative vol-ume rendering, where the mapping of data properties to visual styles can be specified using natural domain language. In Fig. 6c, for instance, contours represent areas of high density; yellow and red highlight regions

with low and very low distances to vessels, respectively.

5.2 Analysis in Multi-variate Data Visualization

Finding interesting structures in multi-variate data is a typical challenge for computational analysis, especially in cases of many variables. Such methods, however, often neglect the semantic meaning of the independent dimensions of space and time. Example methods are aggregation techniques, clustering, regression and outlier analysis [55]. Dimensionality reduction such as PCA or MDS is often applied when analyzing multi-variate data. The data are projected to a lower-dimensional space while preserving their meaningful structures and relationships (see Sec. 3.2). Jänicke et al. [129], for instance, transform multi-variate data onto a 2D point cloud, where data items with similar characteristics are located close to each other. The authors compute a tree where the Euclidean distance between multi-variate data items is minimal. The tree structure is then utilized when transforming the data to 2D. Additional information is encoded using color and point size, and interesting structures can be selected via brushing.

Another analysis challenge with multi-variate data is finding those attributes that represent the most important data characteristics. The grand tour method [47], for instance, automatically generates a sequence of orthogonal projections onto a 2D subspace, which can be used in an animation. Seo and Shneiderman [130] introduce the rank-by-feature framework, where low-dimensional projections such as scatterplots or histograms are ranked based on user-selected criteria (e.g., correlation or entropy). A triangular matrix represents the possible combinations of data variables in a scatterplot and encodes the corresponding ranking score in color. This supports the user to select interesting views on the data. Scagnostics [131] are measures that characterize the point distribution in 2D scatterplots and can be used to detect anomalies in shape, density and trend. Tatu et al. [132] recently propose further quality measures for scatterplots and parallel coordinates that are utilized for ranking these views. Quality metrics can also be used for reordering axes in parallel coordinates in order to find visual structures such as correlations or clusters [48]. In this context, Ward [120] discusses measures for ordering the data attributes that are represented by a glyph.

In order to deal with visual cluttering in parallel coordinates, Johansson et al. [68] utilize clustering and high-precision textures. The number of primitives per pixel are mapped to the pixels' luminance by applying user-defined transfer functions. Each cluster is encoded in color and local outliers are visually enhanced. Novotný and Hauser [69] propose an interactive focus+context visualization for parallel coordinates. The data between each pair of adjacent axes is aggregated in a 2D binmap. Clustering and outlier detection are then applied on the aggregated data in order to show general data trends while preserving outliers. Since these methods are applied in image space (2D binmaps) instead of the original data space, the approach is suitable for interactively rendering larger amounts of data.
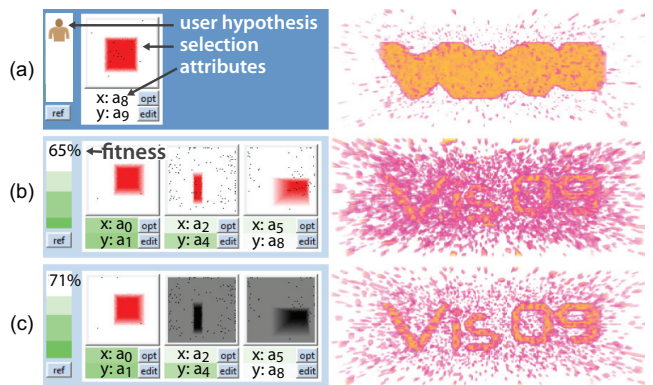

Fig. 7. Combining visual analysis with machine learning [136]: (a) The user specifies an initial hypothesis as a selection on attributes a_8 and a_9. (b) A search algorithm finds alternative hypotheses that explain the same feature but are described by selections on different attributes. The best resulting hypothesis has 65% fitness, where attributes a_0 and a_1 are very important (dark green). (c) The fitness increases when the user deactivates selections (gray) on less important attributes (images courtesy of R. Fuchs, © 2009 IEEE).

Other methods for volume visualization highlight the computed differences or correlations between multiple data variables. Sauber et al. [133], for example, introduce multifield-graphs that give an overview of the correlation between different scalar fields. The user is guided to interesting correlations, which can then be inspected in detail using direct volume rendering. Woodring and Shen [134] propose volume shaders to compare multiple time-dependent scalar volumes by using consecutive algebraic set operators as well as numerical or statistical operators. For interaction and visualization of the resulting volume tree they utilize image spreadsheets (compare to Jankun-Kelly and Ma [19]).

5.3 Interactive Methods for Multi-variate Data

As discussed in section 3.1, multi-variate data are often analyzed in coordinated multiple views. When combining brushing in attribute views with linked 3D volume visualizations, the specified features can be explored in their spatial context too [74], [76], [77]. In the following, we discuss the combination of interactive feature specification with supervised machine learning.

Kniss et al. [114] propose transfer functions for specifying multi-variate features in meteorological data. Interesting data subsets can be selected both in volume and transfer function space using a set of direct manipulation widgets. Tzeng et al. [135] propose an intelligent painting interface that supports the higher dimensional classification of volume data. Regions can be marked directly on sample slices in the volume space, and the data are then classified automatically using a supervised machine learning approach. The training data can then, for instance, be used for classifying other data with similar characteristics. Ma [91] discusses further applications of machine learning and visualization such as flow feature extraction and feature tracking. Fuchs et al. [136] combine interactive feature specification via brushing with machine learning. Using a heuristic search algorithm, the most suitable hypotheses for a user-specified feature can

be identified out of a large search space according to different fitness criteria (see Fig. 7).

6 MULTI-MODAL DATA

Data stemming from different acquisition modalities are common in many physical sciences including climate research, geology, and astronomy [137]. A simulation model can be validated, for instance, by comparing it to the output of another model or measurement data [30]. While multi-variate scientific data are typically sampled or computed for the same spatio-temporal locations, this need not be the case with multi-modal data. Such data can be given on various types of grids (e.g., 2D/3D, unstructured or hybrid) with different time steps and/or spatial resolutions. Accordingly, the different modalities often need to be fused in the visualization, for instance, by resampling them to a common grid [138]. In the medical domain as well, data increasingly often stem from different measurement techniques such as CT, MRI, or ultrasound data. Combining such modalities in a visualization can account for the strengths and weaknesses of the individual ones [139]. The different modalities often need to be registered and normalized to each other in order to make them comparable (see Ardeshir Goshtasby [27] for an overview).

6.1 Representation of Multi-Modal Data

Typical challenges for multi-modal data are the rendering and registration of multiple intersecting scalar volumes, which are possibly sampled at different locations. Similar to multi-variate data, such data can be fused at different stages of the visualization pipeline [23]: 1) during data filtering and visualization mapping, for instance, by reducing the data to relevant features or by resampling to a common grid; 2) during accumulation in the rendering stage; or 3) in image stage, for example, using layering techniques.

Multi-block flow visualization is an example where simulations are performed on multiple grid types with different resolutions [140]. When visualizing the data, these blocks are commonly intermixed at the data level by constructing a common grid. As a result, multi-variate visualization techniques as described in section 5 can be applied. We find, for instance, multi-variate rendering approaches for non-uniform grids [141] or hybrid and non-structured grids [81]. Treinish [138] discusses the data fusion of scattered meteorological observations, for example, by constructing a common grid using Delauney triangulation or resampling to a regular grid. The same author proposes a function-based data model [142] that provides uniform access to different modalities. The model adjusts to the data structure and the way data are processed. Consequently, the same operations can be applied to multi-modal data without resampling to a common mesh or unnecessary interpolation.

Cai and Sakas [143] use the different data modalities as parameters to a multi-volume illumination model (in the visualization mapping stage). As an alternative, the same authors combine color and opacity from different volumes during accumulation, where each volume has it's own transfer function [143]. Similar to that, Grimm et al. [144] fuse multiple intersecting volumes during the rendering by using V-objects, which represent different visual properties of the individual volumes (e.g., illumination, transfer function, region of interest, and transformation). The data are rendered efficiently in software using multi-threading and a brick-wise ray traversal scheme as well as mono-volume rendering for non-intersecting areas. Plate et al. [145] present a framework for rendering large, arbitrarily oriented volumes using slice-based rendering on the graphics hardware. Their approach supports out-of-core techniques and volumes given at multiple resolutions. Lindholm et al. [146] more recently introduce a region-based scene description for GPU-based volume rendering. Using binary space partitioning, the depth information of the intersecting geometry is stored in a view-independent way and time-consuming depth sorting can be avoided.

Beyer et al. [139] present a system for preoperative planning of neurosurgical interventions. Similar to two-level volume rendering [128], the authors render segmented multi-modal data directly on the GPU. Burns et al. [147] combine tracked 2D ultrasound data with illustrative techniques for volume visualization such as flexible cutaways and importance-driven shading. Context information occluding the object of interest can thus be removed and features can be enhanced (compare to importance-driven rendering by Viola et al. [116]).

6.2 Analysis in Multi-Modal Data Visualization

Registration [27] is a typical first step when working with multi-modal data (e.g., using mutual information [28]). A common analysis task is the comparison of multiple data modalities for similarities and differences [30]. According to Verma and Pang [44], scientific data can be compared at the image, data or feature level. Gleicher et al. [45] proposes a complementary taxonomy for InfoVis. The authors distinguish between methods that use juxtaposition, overlay or explicit encoding of differences.

Comparison at the *image level* is the most frequent one. It does not directly operate on the data but on 2D images that result, for example, from a visualization method or from experiments [148]. Examples include side-by-side visualizations (with synchronized viewing conditions) where the user has to mentally relate different images [9], [19], [29], [61]. Other approaches overlay co-registered images, for example, based on a checkerboard pattern or using transparency. Alternatively, per-pixel differences can be directly represent by subtracting the 2D representations from another [107]. For the latter, the selection of an appropriate color map is highly important, for instance, using a diverging map to discriminate positive and negative differences [149]. Zhou et al. [148] present a study of different comparison metrics that numerically quantify image differences between experiments and visualizations. It should be noted that image level comparison usually operates on 2D representations where the intermediate information about how the images were
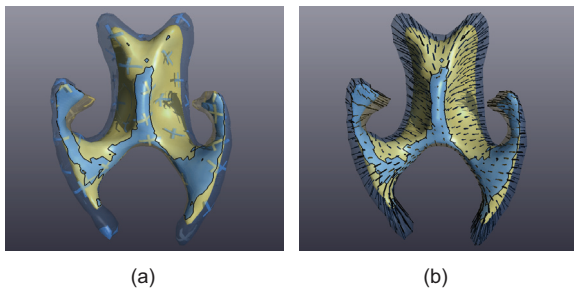
Fig. 8. Comparison of nested surfaces [154]: (a) Transparent surfaces, shadow-casting glyphs, coloring, and contouring are used for comparison. (b) Corresponding points on the surfaces are connected by glyphs (images courtesy of S. Busking).

created is lost. Deviations can, therefore, also result from different visualization settings (e.g., transfer functions, points-of-view, or lighting conditions) and need not necessarily represent data differences [44].

Data level comparison utilizes the raw data as a starting point and often incorporates intermediate information from the rendering process [150]. Sahasrabudhe et al. [151] propose methods for measuring the differences between scalar datasets including spatial and perceptual metrics. Kim et al. [152] propose metrics for data level comparison of direct volume rendering and also incorporate intermediate rendering information in their comparison approach. Malik et al. [153] recently propose the multi-image view that supports the comparison of series of scans from the same specimen.[3] Such approaches are usually superior to pure image level comparison since they include more information and flexibility.

Finally, *feature level comparison* is an extension of data level comparison and is based on extracted features of the data. For flow data, such features can be shock waves, vortices, streamlines, or isosurfaces (see the work of Verma and Pang [44] and Pagendarm and Post [155], for instance). Features from different modalities can be depicted as nested surfaces. Weigle and Taylor II [156], for example, use coloring, transparent textures, and shadow-casting glyphs for visually comparing two nested surfaces. Busking et al. [154] propose an image-based implementation of this approach and add contours where the surfaces intersect as well as local distance cues (see Fig. 8).

6.3 Interactive Methods for Multi-Modal Data

Rendering techniques for multi-modal data often rely on interaction, for example, specifying a transfer function for each data modality which is then combined during rendering [143], [144]. Another challenge with volume rendering is finding a good viewpoint where features are not occluded. This can be done interactively (e.g., by rotating the visualization or using clipping planes) or computationally assisted. Viola et al. [49], for example, utilize mutual information to automatically determine the most expressive viewpoint for a feature, which can

be picked from a pre-defined list. The viewpoint then smoothly changes to give a clear view on the object of interest using a focus+context visualization [116].

7 MULTI-RUN SIMULATION DATA

The previous two sections discuss approaches for a relatively small number of co-located volumes. For comparing such data, for instance, juxtaposed views or isosurfaces can be used [31]. However, the visual analysis of a larger number of concurrent data volumes requires more sophisticated methods. Such data commonly results from multi-run (or ensemble) simulations, which are performed increasingly often in automotive engineering [32], [51] or climate research [12], [31].

Multi-run simulations are an important step in the development of simulation models, where one aims to identify model parameters that have the most influence on the simulation output. In such a *sensitivity analysis* [34], the values of certain model parameters are changed systematically and multiple simulation runs are computed, accordingly. In the resulting data, a distribution of values is given for the same data attribute at each position in space and time (one value for each run). The visualization of multi-run data is especially interesting since it is an alternative approach for representing uncertainty [38], [43]. General approaches for uncertainty visualization are discussed by Pang et al. [157], Johnson and Sanderson [158], and Griethe and Schumann [159]. MacEachren et al. [160], moreover, review approaches for geospatial uncertainty visualization.

7.1 Representation of Multi-run Data

The representation of multi-run data is rather new to the visualization community [33]. It is especially challenging since the data are often higher-dimensional, multivariate, and large at the same time [38]. A direct depiction of many co-located and time-varying volumes of data is often not feasible. Accordingly, the distributions of multi-run values need to be aggregated, for example, by computing statistical summaries [33], [43]. The resulting data can then be visualized using box plots or glyphs, for example. Alternatively, InfoVis techniques such as parallel coordinates or scatterplot matrices can be combined with statistics [31], [161].

Box plots [162] encode important characteristics of data distributions such as minimum and maximum values, mean, median, and other quartile information. Kao et al. [163], [164] extend this approach to 2D multi-run data. In certain cases, the distribution can be represented adequately by statistical parameters such as mean, standard deviation, interquartile range, skewness or kurtosis. The computed statistics are visualized on 2D surfaces using colorcoding and bar glyphs. For other cases, the same authors propose a *shape descriptor* approach. A 3D volume is constructed where the data range is handled as a third dimension and the probability density function (PDF) of the multi-run data is used as voxel values. The peaks in the PDF are then described by a set of shape descriptors

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3. To a certain degree, such dataset series resulting from multiple scans can be considered as multi-run data.
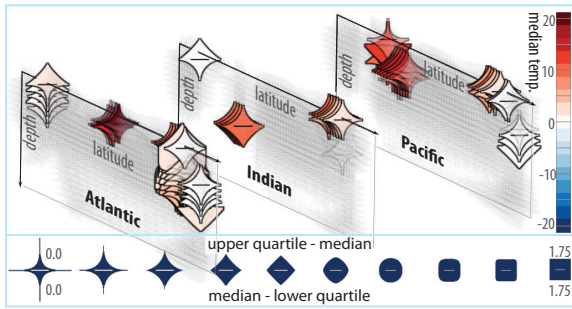
Fig. 9. Glyph-based 3D visualization of multi-run data [37]: Both upper and lower shape represent quartile information by changing from a star (small value), to a diamond, a circle, and a box representing a large value. Glyph size encodes the interquartile range and color shows median temperatures.
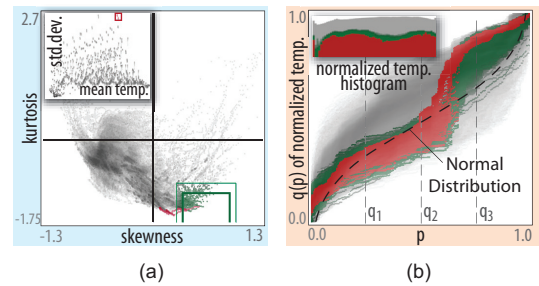

Fig. 10. Relating aggregated and multi-run data of a climate simulation [36], [37]: (a) Interesting statistical properties are brushed and refined in the inset. (b) The corresponding multi-run distributions are emphasized in a quantile plot.

(e.g., number of peaks, height, width, and location), which are displayed on orthogonal 2D slices [164].

Spaghetti plots [42] are utilized by meteorologists to investigate multi-run data, where a contour line is visualized for each run at a selected time step (resembling a pile of spaghetti noodles). Sanyal et al. [165] combine spaghetti plots with a ribbon- and glyph-based uncertainty visualization. The uncertainty glyphs consist of a number of concentric colored circles that represent the standard deviation, interquartile range, and the width of the 95% confidence interval. Potter et al. [35] present a framework for analyzing multi-run data, which consists of overview and statistical visualizations such as trend charts or spaghetti plots. The same authors propose another extension of box plots. The so-called summary plot [43] includes additional statistics of the multi-run data such as skewness, kurtosis and tailing information. These plots, however, cannot be placed in a dense spatial context. Kehrer et al. [37] depict aggregated properties of multi-run data using 2D billboard glyphs that are based on super ellipses (see Fig. 9). The glyphs are carefully designed in order to be placed in a 3D context [123]. Using a focus+context visualization and brushing of aggregated statistics, glyphs that encode certain data characteristics can be interactively explored (see Sec. 7.2).

Chan et al. [166] augment 2D scatterplots by visualizing sensitivity information, which they considered similar to velocities in a flow field. Sensitivities are then represented as tangent lines on the individual points in the flow-based scatterplot. The assumed flow field can also be visualized using streamlines, and data points can be clustered by proximity to these lines. The proposed approach allows the analyst, for instance, to correlate changes in one variable with respect to another one.

7.2 Analysis in Multi-run Data Visualization

As mentioned earlier, statistical methods can be used to reduce the data dimensionality. Kehrer et al. [36], for example, integrate statistical moments (mean, variance, skewness, and kurtosis) into the visual analysis of multi-run data. Traditional and robust estimates of moments as well as measures of *outlyingness* are computed. A moment-based model for the visual analysis is proposed,

which provides guidelines to the multitude of opportunities during such an analysis. Traditional estimates of moments can, for instance, be replaced by robust ones, or the scale of a data attribute can be changed by applying a normalization. For depicting the multi-run data, *quantile plots* that are common in statistics are adapted to enable a focus+context style (see Fig. 10b).

In the visual analysis, multi-run data and aggregated properties are related via an interface [37], which transfers selection information between the data parts.[4] This enables the analyst to work with both data representations simultaneously. Interesting multi-run distributions can then be selected, for instance, by brushing certain aggregated statistics (see Fig. 10a). For the investigated cases with multi-run data and aggregated statistics, the analysis usually starts at the aggregated level [36], [37]. Here, certain data characteristics can be specified via brushing. The feature can then be refined and investigated in detail in the related multi-run data. The analysis can then go back and forth between the data parts, where features are iteratively refined.

As an alternative, mathematical and procedural operators [33] can be applied, which transform the multi-run data into a form where existing visualization techniques are again applicable, for example, streamlines, isosurfaces or pseudo-coloring. The multi-run distributions can be compared against a reference distribution or a single threshold value when drawing contour lines or isosurfaces, for instance. This approach is very promising due to its flexibility. However, the usage of the operators and the interpretation of the resulting visualizations require additional training and care from the user.

Bordoloi et al. [167] apply hierarchical clustering techniques on multi-run data. Data can either be clustered along the spatial dimensions by grouping locations with similar statistical properties and probability density functions of multi-run values—this approach helps to identifying spatial structures and patterns, which may result from the simulated phenomenon. Alternatively, the runs can be clustered base on their similarity. Such an approach supports the comparison of different groups of simulation outcomes, where each group

4. The proposed interface concept is also applicable to other scenarios with heterogeneous scientific data such as multi-physics simulations discussed in section 8.
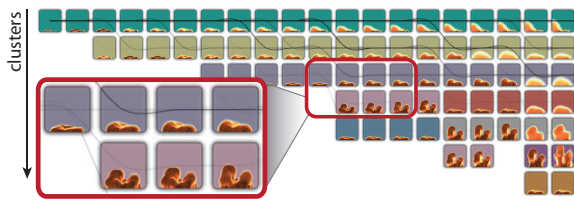
Fig. 11.   Exploration of a multi-run simulation of a visual fire effect [168]: Each run is first split into similar time segments, which are then clustered across the runs. In an overview visualization, each row depicts one cluster with respect to a common time line. The simulation runs are drawn as paths between the clusters (image courtesy of S. Bruckner, © 2010 IEEE).
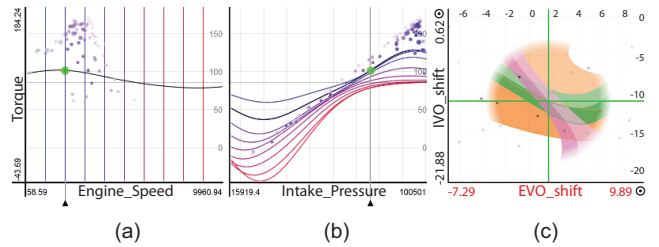

Fig. 12.   Navigating input and output parameters of a multi-run simulation [51], [52]: (a) Variations of an input parameter are indicated with lines. (b) The corresponding changes in the simulation output are predicted and shown as function graphs. (c) The local neighborhood in three output parameters is mapped back to the input parameters, which indicates the sensitivity of the simulation with respect to its input parameters (images courtesy of H. Piringer and W. Berger).

can be represented [167]. In recent work, Bruckner and Möller [168] present a result-driven exploration approach for physically-based multi-run simulations. Each volumetric time sequence is first split into similar segments over time and thereafter grouped across different runs using a density-based clustering algorithm. This approach supports the user in identifying similar behavior in different simulation runs (see Fig. 11).

Correa et al. [169] propose a framework for uncertainty-aware visual analysis. Statistical methods such as uncertainty modeling are incorporated as well as uncertainty propagation and aggregation during data transformations. Approaches for data transformation such as regression, PCA, and k-means clustering are adopted in order to account for uncertainty. A number of views are presented that combine summarized and detailed visualizations of uncertainty. Dependent on the analysis task, uncertain data can be enhanced or de-emphasized.

7.3   Interactive Methods for Multi-run Data

A challenge with multi-run data is the relation of input to output variables of a simulation and vice versa. Nocke et al. [31] utilize coordinated multiple views for analyzing a large number of runs of climate simulations. Statistical aggregations are computed from the runs and visualized using linked scatterplots, graphical tables, or parallel coordinates. The sensitivity of the model to certain input parameters can be explored via brushing, and the related model runs can be compared in detail (compare to a similar approach on injection systems simulations [32]).

Certain methods that were originally designed for multi-dimensional data can be used for multi-run data as well. HyperSlice [170], for example, represents a higher dimensional function as a matrix of orthogonal 2D slices around a user-controlled n-dimensional focal point. The Prosection Matrix [171] extends this concept by projecting also the local neighborhood of the slices to 2D scatterplots. The approach supports also filtering via brushing. HyperMoVal [51] builds upon these concepts and enables the interactive visual validation of surrogate models. Such models are based on statistical regression and approximate the output of a more time-consuming simulation. HyperMoVal utilizes 2D and 3D projections of multi-run data around a user-controlled focal point. Model predictions of variations of one input parameter are represented as families of function graphs (see

Fig. 12b). The predictions can then be compared to known results of the multi-run simulation (shown as points in the Figs. 12a and 12b). The approach supports, for example, the identification of regions with bad fit.

Berger et al. [52] extend HyperMoVal for exploring the continuous space of input and output variables of the simulation. The local neighborhood around the focal point in the input parameters is mapped to the output domain using k-nearest neighbor estimators or linear regression models. Since a direct mapping from output to input parameters of a simulation is not possible, a "spyhole" approach is proposed. In Figure 12c, the local area around the focal point is shown where variations of input parameters do not affect the predicted output by more than a certain threshold. Also, the uncertainty of the prediction can be visualized using box plots.

Matković et al. [41] visualize multi-run data as families of data surfaces with respect to pairs of independent data dimensions. Using multiple linked views and brushing, the authors analyze projections and aggregations of the data surfaces at different levels (e.g., a 1D profile or single aggregated value per surface). The same authors propose a visual steering approach [172] where new simulation runs are triggered by interactively narrowing down the control parameters in the visualization via brushing. This approach realizes a tight combination of interactive visualization and computational simulation.

In later work, Matković et al. [173] propose the simulation model view which is directly integrated in their coordinated multiple views framework. The view represents the building blocks of the utilized simulation process and model at three different levels of detail (using a histogram, scatterplot or curve view). The approach aims at bridging the gap between the simulation model and resulting multi-run data. Unger and Schumann [174] present a similar framework that facilitates the understanding of simulation processes at different levels. The user can compare and simultaneously explore the underlying data model, different parameter settings for the simulation, as well as individual runs or aggregated multi-run values.

We clearly see a lot of potential for future research on multi-run data. This kind of data is gaining increasing importance due to the technological developments in

climate research, engineering, and other fields. Visualization must deal with multi-run data that are also multi-variate and spatio-temporal. It is not at all straightforward to visualize an overview of several hundred runs of time-dependent 3D data. Advanced data abstraction and aggregation techniques are required that are aware of data trends and outliers.

8 MULTI-MODEL SIMULATION DATA

Data from multi-model simulations have been rarely addressed in the visualization community so far. Such simulations, however, are gaining importance in areas such as multi-physics or climate research [11], [12]. In the climate system, for instance, different compartments such as ocean, ice, surface, and atmosphere are interacting with each other. Ocean and atmosphere exchange through thermal absorption, precipitation, and evaporation, also ice and air are interacting. Accordingly, ocean and atmosphere models are often coupled in the simulation [12]. The models are often not computed on the same types of grid, or for the same time steps. When analyzing feedback between these models, statistical aggregates are usually investigated. Fluid–structure interactions (FSIs), to address another example, are interactions of a deformable or movable structure with an internal or surrounding flow [11]. They are among the most important and—with respect to both modeling and computational issues—the most challenging multi-physics problems, and therefore currently a hot topic in simulation research itself. The variety of FSI occurrences is abundant and ranges from bridges, flexible roofs, or off-shore platforms to micropumps and injection systems, from parachutes via airbags to blood flow in arteries or artificial heart valves, to name just a few [11].

For visualization research it is very challenging to generate a coherent representation from such data, for instance, when one model is simulated on a 2D grid and the other one on a 3D grid. How can different attributes given in the different models be compared to each other? How can data be represented, where there are values missing (e.g., an attribute is simulated in one model but not in the other, or the data are not uniformly available for a spatial dimension). Also, how can selections and features be communicated between different models, especially when these are given on non-overlapping grids or different time steps? One is, for example, interested in the areas of an ocean model that are influenced by adjacent atmospheric regions exhibiting certain characteristics such as high temperatures. How can such a feature from the atmosphere be propagated to the ocean part?

Kehrer et al. [37] recently propose a concept that integrates and relates two parts of scientific data in the visual analysis. The fractional degree-of-interest (DOI) attribution of the data, resulting from smooth brushing [80], is utilized as a common level of data abstraction between the related parts. As an example, a fluid–structure interaction of warm water flow though a cooler aluminum foam is investigated. Similar to the simulation, an *interface* is created that relates individual
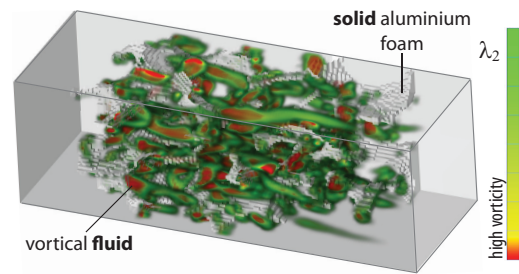

Fig. 13. Visual analysis of heat transfer between the fluid and solid part of a multi-physics simulation [37]: Both data parts are related via an interface that enables a bidirectional transfer of features. Vortical flow is selected via brushing. The feature is automatically transferred to the solid part, where it is further analyzed and related to other features.

grid cells between the two data parts (see Fig. 2). The interface enables the bidirectional transfer of DOI information. For understanding flow characteristics such as heat exchange, vortices are highly important. Vortical regions are thus selected via brushing in the fluid part of the data (see Fig. 13). The corresponding feature is instantly transferred to the foam part via the interface. Here, it can be related to other features specified in the solid part. The interface enables the investigation of a direct relation between turbulent flow around the foam structure and a corresponding heating in the foam.

To the best of the authors' knowledge, this work [37] is the first step into the direction of visual analysis of multi-model scenarios. Since the related simulation are becoming increasingly popular in the application domains, we see a great potential for future visualization research here.

9 DISCUSSION AND OUTLOOK

The majority of the approaches discussed in this survey specifically address one or two facets of scientific data. What is often missing are general concepts for handling the heterogeneity of multi-faceted data (e.g., multi-run data are often spatio-temporal and multi-variate as well). One possible solution are coordinated multiple views, which combine and link well-known visualizations for different kinds of data. In such a framework, for example, function graphs can be used to analyze time-varying data, volume rendering for spatial data, 2D scatterplots or parallel coordinates for multi-variate data, or glyphs and box plots for encoding summary statistics of multi-run data. A challenge in this context is the relation of multiple views, allowing the investigation of features across data facets, datasets, as well as levels of data abstraction [9], [37], [74], [75], [115]. Context-preserving visual links [175], for example, interconnect related pieces of information across views and applications.

Another challenge is the extraction of meaningful information from heterogeneous scientific data. Such data can be fused on the data level, for example, by resampling or by using a data model that provides unified access to different modalities [142]. Another option is to fuse multi-faceted data on the feature level, for example, by exchanging selection information across different data

parts [37], [75]. The data markups then represent the first level of semantic abstraction, ranging from raw data to knowledge [56]. This abstraction to the feature level enables the joint integration of heterogeneous data parts. Features can be exchanged between parts that are given on different levels of aggregation (e.g., multi-run and aggregated data) or on various types of grids [37]. Such a semantic abstraction is especially useful, since domain scientists usually think in application terms instead of data terms (e.g., objects or phenomena).

One interesting observation from our study was that many overview articles discuss approaches according to the different stages in the visualization pipeline (e.g., multi-variate data fusion [23], comparative visualization [44], [45], or quality metrics [48]). Analytical methods can, for example, be applied before the visualization mapping (in data space). Alternatively, they can control the visualization mapping or measure the quality of the resulting image [48]. Also, the user can interactively control the settings at different stages of the analysis pipeline [59]. Especially the combination of computational analysis and interactive visualization methodology—as proposed in the visual analytics agenda [4]—is a promising direction, and we expect to see a lot of more interesting work in this area. Examples are feature-based approaches that (semi)automatically extract interesting patterns from the data [74], [75], [129]. Recently, May [176] presented a thoroughly structured overview of different opportunities for integrating interactive and computational means in visual analytics. One important step in this context is the integration of machine learning methods that can learn from previous user input and data, and configure the parameters of the visualization based on the acquired knowledge [56], [91].

As another observation, we see a gap between the techniques used by domain scientists and the approaches available from visualization research. Recent advances in visualization are rarely used in application domains such as climate research (compare to Nocke et al. [177]). One reason for this may be that systems are complex to use and can overwhelm the user with a multitude of options and parameters. Also, it is not always obvious how such methods integrate into the typical workflow of the domain. A major challenge for future developments is thus to further bridge this gap, for example, by including knowledge from domain experts when designing visualization solutions [2]. Visualizations should follow guidelines from perception research and human–computer interaction [39], providing simple graphical user interfaces and advanced visualizations [59].

In general, current approaches rarely address the heterogeneity of multi-faceted scientific data. We see here a definite need for novel concepts and methods and thus see it as a promising research direction in visualization.

10 CONCLUSIONS

The visualization and interactive visual analysis of multi-faceted scientific data are gaining increased importance in areas such as engineering, medicine or climate research. This is due to the fact that computational power increases rapidly, measurements are getting more accurate and detailed, and multi-modal data are becoming more common. Accordingly, also model and data scenarios are getting more complex. Data are often multi-variate, spatio-temporal and stem from multi-modal, multi-run, and/or multi-model scenarios. Visualization has been well established to explore and analyze single facets of such data and to communicate results from data analysis. With respect to multi-faceted scientific data, however, we see a variety of interesting challenges that require advanced visualization technology. In this survey, the related state of the art has been discussed. A categorization of approaches has been proposed that is based on common visualization, interaction and analysis methods. What is largely missing are approaches that address a multitude of facets of scientific data.

We identify, in particular, the visualization and analysis of data stemming from multi-run simulations and interacting simulation models (e.g., coupled climate models or multi-physics simulations) as rewarding directions for future research, as well as multi-modal visualization. A challenge is to jointly integrate larger amounts of concurrent data volumes in the visual analysis, possibly given on different grids and/or with different data dimensionality [37]. Another challenge is how to investigate feedback between interacting compartments of the simulation. For multi-variate and time-dependent data, we can find a lot of related work that brings up good solutions. The visualization and analysis of these kinds of data belong to the top challenges in current visualization research [2].

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