



Visualization for the Physical Sciences

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Abstract

Close collaboration with other scientific fields is an important goal for the visualization community. Yet engaging in a scientific collaboration can be challenging. The physical sciences, namely astronomy, chemistry, earth sciences and physics, exhibit an extensive range of research directions, providing exciting challenges for visualization scientists and creating ample possibilities for collaboration. We present the first survey of its kind that provides a comprehensive view of existing work on visualization for the physical sciences. We introduce novel classification schemes based on application area, data dimensionality and main challenge addressed, and apply these classifications to each contribution from the literature. Our survey helps in understanding the status of current research and serves as a useful starting point for those interested in visualization for the physical sciences.

Keywords: scientific visualization, visualization

ACM CCS: I.3.8 [Computer Graphics]: Applications–Visualization; I.6.6 [Simulation and Modeling]: Symulation Output Analysis–Visualization; J.2 [Physical Sciences and Engineering]: Astronomy–Visualization; J.2 [Physical Sciences and Engineering]: Chemistry–Visualization; J.2 [Physical Sciences and Engineering]: Earth and atmospheric sciences–Visualization; J.2 [Physical Sciences and Engineering]: Physics–Visualization

1. Introduction and Motivation

In his influential work, Lorensen [Lor04] reflects on the decrease in the rate of introduction of new techniques in the field of visualization. Lorensen warns of the eventual death of visualization unless proper measures are taken. He advocates a range of measures that can be implemented by the IEEE Visualization Organizing Committee and by the visualization community. He proposes three main directions in which the field of visualization could regain a healthy state: (1) close collaboration with customers can pose challenging problems and expose our community to new and exciting application areas, (2) alliances with other fields, especially computer vision and structural analysis, can generate new synergies and (3) the identification of some grand challenges could energize our community.

The first proposition provides the motivation for this survey. We review application papers on the physical sciences, classify them in related categories and use the result to identify fields where visualization has been used extensively and fields that may benefit from further exploration. Our literature survey places special emphasis on recent literature as well as citation rates.

Ertl [Ert10] argues that the field of visualization is flourishing due to the overall growth of the number of submissions to the main Visualization, Information Visualization and Visual Analytics conferences, and the recent Visual Analytics initiatives in the United States and Europe. In discussing the future of the visualization field, Ertl points out that many visualization techniques are not usable in practice, due to the complexity of their application, and that standard datasets

may not be useful for driving research towards relevant applications.

Ertl's presentation outlines possible drawbacks of not collaborating with application scientists and provides further motivation for our survey. Physical scientists study many interesting phenomena that pose new and exciting challenges to visualization researchers. We identify the dimensionality of the data used to study the underlying phenomena, the main challenge addressed by each paper in our survey, describe the novel techniques used to address those challenges and classify the papers based on data dimensionality and these challenges.

The main benefits and contributions of this paper are:

1. We review visualization work for the physical sciences published in the last 10 years.
2. This is the first survey of its kind that provides a comprehensive view of existing work on visualization for the physical sciences.
3. We introduce novel classifications schemes based on application area, data dimensionality and challenges addressed, and apply this classification scheme to each contribution.
4. Our classification helps in understanding the status of current research by highlighting mature areas in visualization for the physical sciences and areas where few solutions have been provided. Collaborations with domain scientists have the potential to introduce new problems to the visualization field and can contribute to its advancement.

This is not simply a list of papers. We also explore and describe the relationship between papers. Each paper's contributions are presented in the context of closely related work following a specific methodology [Lar11].

The rest of the paper is organized as follows: we define the scope of the survey in Section (1.1) and we further motivate our paper (Section 1.2); we describe our classifications (Section 2), we review visualization papers for astronomy (Section 3), for chemistry (Section 4), for earth sciences (Section 5) and for physics (Section 6), and we end with conclusions (Section 8).

1.1. Scope and methodology

This survey reviews visualization papers for the physical sciences. According to the Encyclopædia Britannica [bri10f], physical sciences study the inorganic world whereas biological science studies the organic (living) world. Visualization papers on biology are beyond the scope of this paper. Engineering, defined as the application of science to the conversion of the resources of nature to the uses of human kind [bri11b], is also beyond the scope of our survey. Physi-

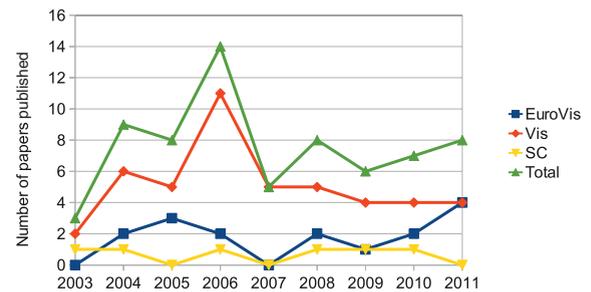


Figure 1: Number of papers published at the Vis, EuroVis and Supercomputing conferences on physical science applications.

cal sciences include astronomy, chemistry, physics and earth sciences.

We do not include flow visualization papers as most are engineering, many are technique rather than application papers (that is, they solve known problems rather than new problems so the domain science description is short or non-existent) and there are already many surveys on flow [MLP*10, PL09, LHD*04].

Our survey includes application papers rather than technique papers. Consequently, we include papers that present background information about a target domain, describe research questions, and in some cases, include a case study documenting insights found by the users. Although for the review process, papers are labelled as application or technique, no such label exists after publication. Consequently, our decision to categorize a paper as application or technique is driven by the criteria above.

We review visualization papers on physical sciences published at the IEEE Visualization (VIS), EuroVis and Supercomputing (SC) conferences and IEEE Transactions on Visualization and Computer Graphics (TVCG) and EG Computer Graphics Forum (CGF) in the last 9 years (Figure 1). Because data in the physical sciences have an inherent spatial placement whereas infovis addresses abstract data [vHMM*11, Tel08], application papers for the physical sciences are not normally published by the InfoVis conference. This fact is confirmed by our search through the last 10 years of the InfoVis proceedings. This does not mean that infovis techniques are not used for research in the physical sciences. On the contrary, there are many examples of papers where techniques from both scientific visualization (scivis), that deal with spatial data, and infovis are used to solve problems in the physical sciences both in the computer science [RPW*08, QCX*07, BWH*11] and in the domain specific [CPB*08, JMS*07, BJJ*07] literature. We also include references to survey papers in domain-specific areas [HF11, KR08, EYD01, Val06].

For consistent paper summaries we incorporate a specific methodology described by Laramee [Lar11].

1.2. Visualization for the physical sciences

The broad aim of research in the physical sciences is to make sense of the world around us. That is, to measure quantities of some physical system, derive a model based upon the result and then test the model to see whether it can make useful predictions. The first and last steps usually require the collection, assimilation and comparison of large quantities of data. The task of understanding the data and making comparisons between different but allied data is where the visualization community has a role, especially given that most physical systems are three-dimensional and time-dependent. That is not to say that researchers in the physical sciences are incapable of understanding their data on their own—they are, and if the methods of the visualization community were explained to them, they could honestly describe themselves as good practitioners of the subject. Yet, there are many challenges [Joh04, RK07] which require time and effort, and pose obstacles that a physical scientist may not wish, nor be able, to tackle. Off-the-shelf visualization packages, though a great first step in visualizing data, may fail to meet some of the challenges listed by Johnson. Even more importantly, visualizing data in the physical sciences may require domain specific knowledge that would be difficult to provide in a general purpose visualization package. For these reasons visualization scientists have the opportunity to significantly influence future discoveries and drive innovation in the physical sciences.

We view applications as a means to introduce areas with new problems and new solutions to the visualization community. Once a problem is well described and proves important and challenging, other visualization researchers may study it without the need for a close collaboration with the application scientists. Eventually, significant research is accumulated that handles previously introduced, well described problems so that those problems can be solved.

Close collaboration with other scientific fields is seen by leading researchers in visualization [Lor04, Joh04, Ert10, JMM*06] as an important goal for the visualization community. Through these collaborations, the visualization community can be exposed to exciting new application areas and can be asked to solve challenging problems. In this way the visualization community can develop innovative techniques to solve our customers' problems and keep the visualization field vibrant and relevant in the future.

Our survey contributes to this goal by reviewing many recent visualization papers for the physical sciences, by comparing and contrasting them, pointing out how they relate to one another and by classifying them to highlight mature areas where visualization has made many contributions and suggest areas where more visualization work can be done.

2. Classifications and Overview

Classifying visualization literature in the physical sciences is non-trivial given the many sciences covered, the diverse domain specific knowledge required, and the varied visualization techniques used.

We classify the reviewed papers based on the area of physical sciences they address: astronomy, physics, chemistry and earth sciences. Given that each of these broad areas is divided into many different fields and sub-fields, and that some of these fields are overlapping, papers can be classified in more than one area. For instance, molecular dynamics visualization papers might be classified as chemistry or biology, depending on the nature of the molecules under consideration.

We have two goals for our classifications: (1) We want to provide a quick but comprehensive picture of the main contribution of each paper and (2) we want to present the state of current research, which may in turn help in deciding a future research direction.

A typical classification of visualization techniques [Tel08] (scalar, vector, tensor, ...) fails to fulfill these goals. On one hand, most of the papers reviewed visualize scalar data, which means that we would not get a good distribution among categories. On the other hand, the fact that many papers use scalar visualization techniques does not necessarily mean that these techniques should not be used to visualize data in the future.

We provide two alternate classifications of the literature. We categorize the literature based on data dimensionality and the generic main challenge they address [Joh04]. These challenges highlight the main contribution of the paper and convey useful information about the work (such as making use of 'graphics hardware' or using 'feature detection') not available in other visualization taxonomies (see Ward *et al.* [WGK10] for a summary of existing visualization taxonomies). If the data studied covers more than one dimension, we choose the higher dimension for classification. If a paper addresses more than one challenge, we choose the main challenge addressed by the paper. We present a short description of challenges addressed by papers in our survey; see the work by Johnson [Joh04] for a detailed description of these and other major visualization challenges.

1. **Multi-field visualization.** Often physical data contains several attributes for the same point in space. The ability to effectively visualize multiple fields simultaneously so that it facilitates the analysis of the relations and correlations between those fields is the goal in this category.
2. **Feature detection.** Modern sensors and computers produce and store data measured in giga to terabytes in size. Locating features of interest in these vast amounts of data, representing them and tracking the evolution of features in time and/or space are the main goals in this category.

3. **Graphics hardware.** Scientific data may be too large to process and render in real time. The papers in this category propose novel ways to use the available graphics hardware (GPUs) to address these challenges.
4. **Modelling and Simulation.** Visualization application papers are defined by the fact that they solve domain specific problems and use domain specific knowledge. We include in this category papers that use the science in their respective fields to model, simulate and visualize physical phenomena, for which advanced domain knowledge is needed. This category is more specific than the original Johnson challenge ‘think about the science’ which should apply to all application papers.
5. **Scalable visualization.** The large amounts of data analysed by scientists can be challenging on several levels: data may be too large to read, process or visualize at interactive speeds. Papers in this category use algorithms that take advantage of available (parallel) I/O, processing and visualization resources to produce scalable visualizations that are able to visualize larger datasets as the amount of resources is increased. We define this challenge similarly to Chen *et al.* [CHHK11]. This is an extension of the original Johnson challenge ‘scalable, distributed and grid-based visualization’ as it includes visualization papers that address any of the challenges created by large data: I/O, processing and visualization, whereas the original Johnson challenge focuses on the last one.
6. **Error/uncertainty visualization.** Acquisition or simulation errors/uncertainty are part of the data analysed by physical scientists. In addition, errors are introduced by data transformation (through resampling, filtering, quantization and rescaling) and visualization [JS03]. The main focus for papers in this category is integration of error visualization into the main visualization of data.
7. **Time-dependent visualization.** A common way of visualizing time-dependent data is by rendering a frame for each time step and assembling those frames in a video. Papers in this category aim to address the main drawback of presenting time-dependent visualizations through a video: the inability to engage in interactive exploration of the data.
8. **Global/local visualization (details within context).** The techniques in this category aim to integrate a visualization of the whole data required for navigation and a global understanding of the phenomenon described with selection and detailed visualization of sub-sets of interest.
9. **Comparative visualization.** Comparative visualization refers to the process of understanding how data from different sources are similar or different [VfETV, PP95]. Such analysis can happen at different levels: image, data, derived quantities and methodology levels. The two sources can be compared by using two visualization images shown side by side, superimposed

or as two symmetrical halves (image level); directly comparing the available data fields (data level); comparing derived quantities such as features in the data (derived quantities level) or quantifying the differences in experiment, simulation or visualization parameters (methodology level).

Other major visualization challenges discussed in [Joh04], but not included in our survey are: ‘Perceptual Issues’, ‘Human–computer interaction’, ‘Integrated scientific and information visualization’, ‘Visual abstractions’ and ‘Theory of visualization’. Some of these challenges (perceptual issues, quantify effectiveness, human-computer interaction, visual abstractions and theory of visualization) are mostly addressed by papers not associated with a physical science or (integrated scientific and information visualization) are too abstract to be used to define a main challenge of a paper. Comparative visualization challenge is not in the list presented by Johnson [Joh04], however, it is the focus of a paper in our review and is identified as a technique needed by application scientists by a major visualization research initiative [VfETV].

Table 1 presents an overview and classification of visualization work on the physical sciences. Papers are grouped by domain along the columns and by the temporal and spatial dimensionality of data along the rows. Entries are also ordered chronologically within each sub-group. This table highlights the dimensionality of the data for which most of the surveyed work has been done.

Table 2 presents an alternate classification for visualization work for the physical sciences. Papers are grouped by domain along the columns and by the main challenge or contribution along rows. Each entry is coloured according to the temporal and spatial dimensionality of the data. Entries are also ordered chronologically within each sub-group. This table highlights the main challenge addressed by each work, and provides a starting point for exploring areas of future work.

We review a number of solutions designed to address the **multi-field visualization** challenge. Multi-field 2D data is visualized using a field [LFH08] or using time [YXG*10] as a third dimension. Multi-field 3D data is visualized using glyphs and a variation in the glyph colour [SIG05] or shape [CFG*05, BvL06, JKM06, DMB*06, MDHB*07], using trajectories, vector glyphs or surfaces together with volume rendering [SYS*06, JCSB03], parallel coordinates [QCX*07] or multiple-linked views and brushing [CFG*05, KLM*08].

Auralization is the technique of creating audible sound files from numerical data [Vor08]. Perception of sound depends on many parameters such as the type of source, direction of sound, source movement, listener movement and environment. Auralization is used to enhance visualization of multi-field data by mapping various fields to sound and

Table 1: A classification of visualization research in the physical sciences by domain along the columns and by the dimensionality of the data along the rows. Entries are ordered in chronological order within each group. The colors show the main challenge addressed by each paper: *multifield vis.*, *graphics hardware*, *feature detection*, *scalable vis.*, *time-dependent vis.*, *uncertainty/error vis.*, *global/local vis.*, *comparative visualization*, and *modeling and simulation*. This table provides a quick overview of research and highlights the dimensionality of the data where most recent work has been done.

Dimensionality		Astronomy	Chemistry	Earth Sciences	Physics
Spatial	Temporal				
	static	[LFH08]			
2D	time-dependent			[QCX*07] [JBMS09] [KGH*09] [YXG*10] [SZD*10] [MNV10] [DBS*11]	[LLCD11]
	static	[MKDH04] [MHLH05] [MQF06] [LFH06] [LFLH07] [FSW09]	[BDST04] [MHM*04] [CS04] [CS05] [QEE*05] [TCM06] [JV09] [LBH11]	[PGT*08]	[LCM*05] [WBE*05] [JKM06] [MJK06] [SCT*10] [TGS11]
3D	time-dependent	[SB04] [NJB07]	[SIG05] [QMK*06] [BGB*08] [KBE09] [LBPH10] [KFR*11] [BWH*11]	[REHL03] [MSB*03] [JCSB03] [YMW04] [SFW04] [SBS*04] [SYS*06] [TYRG*06] [KLM*08] [WHP*11]	[SBSH04] [CFG*05] [BDM*05] [RE05] [DBM*06] [SPL*06] [LBM*06] [BvL06] [DMB*06] [MDHB*07] [LCM07b] [RPW*08] [BMD*08] [GB08] [CLT*08] [GMDW09] [MGW10] [GRDE10]

Table 2: An overview and classification of visualization research on the physical sciences. The classification is based on [Joh04]. Papers are organized by domain along columns and by the main challenge addressed along rows. Rows are in decreasing order based on the number of contributions. Each entry is also colored according to the dimensionality of the data. We use cold colors for 2D data and warm colors for 3D data. The colors show 2D static, 2D time-dependent, 3D static and 3D time-dependent data. Finally, entries are ordered in chronological order within each group. This table provides a quick overview of research in the physical sciences.

Visualization Challenge	Astronomy	Chemistry	Earth Sciences	Physics
Multifield visualization	[SB04]	[SIG05]	[JCSB03]	[CFG*05]
	[MHLH05]		[REHL03]	[JKM06]
	[LFH08]		[SBS*04]	[BvL06]
			[SYS*06]	[DMB*06]
			[QCX*07]	[MDHB*07]
			[KLM*08]	
			[YXG*10]	
Feature detection	[MQF06]	[MHM*04]	[PGT*08]	[SBSH04]
	[NJB07]	[BGB*08]	[JBMS09]	[MJK06]
		[LBH11]	[WHP*11]	[SPL*06]
		[KFR*11]		[LBM*06]
		[BWH*11]		[SCT*10]
Graphics hardware		[BDST04]		[LCM*05]
		[QEE*05]		[RE05]
		[TCM06]		[GMDW09]
		[JV09]		[MGW10]
		[KBE09]		[GRDE10]
Modeling and simulation	[MKDH04]		[CS04]	[WBE*05]
			[CS05]	[BDM*05]
Scalable visualization	[FSW09]	[QMK*06]	[MSB*03]	[LCM07b]
			[SFW04]	[GB08]
			[YMW04]	[CLT*08]
			[TYRG*06]	[BMD*08]
			[KGG*09]	
			[MNV10]	
Error/uncertainty visualization	[LFLH07]	[SZD*10]		
Time-dependent visualization			[DBS*11]	[LLCD11]
Global/local visualization	[LFH06]			
Comparative visualization				[DBM*06]

source characteristics [SB04]. Although this is an appealing idea, many challenges remain, such as meaningful mapping between field values and sounds, generating pleasant sounds and the speed of processing.

Realistic visualization of physical phenomena use multi-field data from simulation or acquired through non-visual means and aim to visualize this data in a visually accurate way. Examples include: visualization of storm and cloud scale simulation data [REHL03]—these visualizations appeal to meteorologists, who are trained to extract information about a forming storm through visual observation; visualizations of hot fluids discharges from seafloor vents acquired using sonar scans—these visualizations may be used for comparison with data acquired with video cameras [SBS*04]; or visualizations of nebula's dependence on viewpoint and dust distribution [MHLH05]—these visualizations can be used for producing scientifically accurate animations for educational purposes or for exploring the visual effects of changing a nebula's physical parameters.

Papers that present **feature detection** as their main goal are varied. Locating important features within the data requires domain-specific knowledge. We review techniques that examine structures defined by intercluster galaxies [MQF06] and visualize the build-up regions of ionized gas around the first stars [NJB07]. We survey papers that detect anomalous structures in molecular dynamics simulation data [MHM*04] or in nematic liquid crystals [MJK06, SPL*06], visualize optical power flow through nano-apertures around critical points [SBSH04], determine the topology of a toroidal magnetic field [SCT*10, TGS11], determine states of energy minima and represents relationship between these states in a chemical system [BWH*11], calculate the lines that separate rocks with different mineral densities or porosity characteristics [PGT*08], identify regions in the atmosphere which can act as indicators for climate change [JBMS09], calculate paths of molecules to possible binding sites [LBH11] and detect mesoscale eddies in an ocean simulation [WHP*11]. Three papers approach both feature detection and feature tracking: Bidmon *et al.* [BGB*08] track and visualize the paths of solvent molecules, Krone *et al.* [KFR*11] track protein cavities and Laney *et al.* [LBM*06] identify and track the surfaces separating a heavy fluid placed on top of a light fluid.

Most papers that use **graphics hardware** (GPUs) are from chemistry or physics and visualize molecules [BDST04, RE05, TCM06, GRDE10], molecular surfaces [KBE09, LBPH10], or quantum chemistry simulations [QEE*05, JV09]. In physics, Grave *et al.* [GMDW09] visualize the Gödel universe, Müller [MGW10] presents computer simulations exploring the special theory of relativity and Laney *et al.* [LCM*05] describe a hardware accelerated simulation of radiographs.

Papers in the **modelling and simulation** category make use of domain specific knowledge to model, simulate and

visualize physical phenomena. We review simulations of sound reflection and refraction within a room [BDM*05, LCM07b, CLT*08, BMD*08, DBM*06] and works that model and visualize theories of general and special relativity [WBE*05], the Gödel universe [GB08], planetary nebula [MKDH04] and the molecular skin surface [CS04, CS05]. These papers take advantage of advanced domain knowledge and/or close collaboration with the physical scientists to advance the science in the physical and visualization fields.

Works in the **scalable visualization** category address I/O, processing and/or visualization challenges caused by large data. Solutions include a remote hardware-accelerated visualization farm [QMK*06], a public-resource climate modelling [SFW04], adjusting the frequency of the output from the simulation based on application and resource dynamics [MNV10], using parallel I/O and query-driven visualization [KGH*09, RPW*08], using parallel I/O [YMW04] and parallel visualization [MSB*03, YMW04] and designing all components of the simulation pipeline (problem description, solver and visualization) so that they execute with shared data structures and no intermediate I/O [TYRG*06]. Fraedrich *et al.* [FSW09] visualize large particle-based cosmological simulations using a multi-resolution hierarchy and techniques designed to reduce disk and display limitations produced by the large data.

Li *et al.* [LFLH07] present tools and techniques for visualizing **error and uncertainty** in large scale astrophysical environments and Sanyal *et al.* [SZD*10] visualize the uncertainty associated with weather prediction.

Two papers address the **time-dependent visualization** challenge. Drocourt *et al.* [DBS*11] present a radial visualization using nested rings to show the evolution in the temporal dimension, whereas Lipša *et al.* [LLCD11] address the large fluctuations in attribute values by computing the average of values for a time window behind the current time step.

There is one paper that has as its main challenge **global/local visualization (details within context)**. Li *et al.* [LFH06] present a set of techniques to facilitate travel and context acquisition in an astronomic virtual environment. Often papers [KLM*08, CFG*05, LFH08, YXG*10, RPW*08] that visualize multi-field data include multiple linked views and interactive brushing which can show both a context and a focus view. Global/local visualization is, however, secondary in these cases.

There is one paper [DBM*06] that focuses on **comparative visualization** of two different approaches for acoustic simulation.

The next sections review visualization papers for astronomy, chemistry, earth sciences, and physics. Note that, to address space limitation, we only include full summaries for a subset of the reviewed papers. Papers that include a full summary are indicated with a star next to their citation.

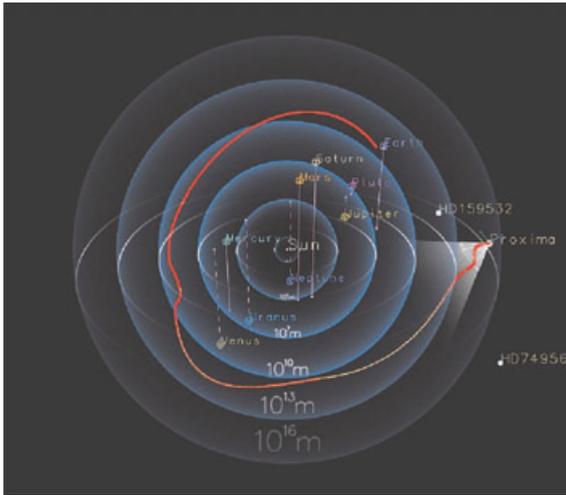


Figure 2: Planning a travel path from Centauri Proxima (10^{17}) to Earth (10^{11}) using logarithmically mapped eye space [LFH06]. Image courtesy of Philip Fu.

3. Astronomy

Astronomy is the science of the entire universe, which includes the study of planets, stars, galaxies, nebula and interstellar medium. Astronomy and physics are linked through cosmological theories based on the theory of relativity [bri10a].

This section includes papers that describe visualizations of nebula [MKDH04]*, [MHLH05]* and a paper that presents an auralization of cosmological explosions [SB04]*. Included are papers that visualize inter-cluster regions inside galaxy clusters [MQF06]*, present an interactive exploration of the visible universe [LFH06], visualize uncertainty in astrophysical data [LFLH07], visualize the formation of the first stars [NJB07], visualize multi-wavelength sky data [LFH08]* and cosmological simulations studying matter distribution in the universe [FSW09].

For further reading on the current state-of-the-art of visualization in astronomy and future directions for visualization see Hassan and Fluke [HF11], Kapferer and Riser [KR08] and Goodman [Goo12].

The visible universe spans a huge range of distances, and contains mostly empty space. These characteristics make it difficult for users to navigate and gain understanding of position and orientation in a virtual environment simulation of the visible universe. Li *et al.* [LFH06] present a set of techniques to facilitate travel and context acquisition in an astronomic virtual environment (Figure 2).

Navigation and object representation in the multi-scale universe is done using power spatial scalling [FH07]. This technique scales the entire Universe's data relative to the cur-

rent view scale. The authors use a 3D compass for orientation reference and annotated 3D landmarks for context. They use a cube, cylinder or sphere as power cues to show the current image scale, and use an edge which fades in when an object is close to the viewpoint as a proximity cue. Li *et al.* [LFH06] use a slice of the sky flattened into a 2D chart and a map of the entire universe scaled logarithmically relative to a certain view scale as an overview map. Li *et al.* [LFH06] extend their previous work [FH07] with techniques that facilitate travel and context understanding in an astronomic virtual environment. The phenomena studied is 3D, static and the main challenge is global/local visualization (details within context).

Li *et al.* [LFLH07] present tools and techniques for visualizing uncertainty in large scale astrophysical environments. These techniques raise awareness and comprehension of the large positional uncertainty that exists in astrophysical data. This uncertainty in spatial quantities such as distance and velocity is caused by the limited precision of the standard astronomic measurements of parallax, proper motion, and radial velocity. Presented tools for visualizing uncertainty include: a unified colour coding scheme for log-scale distances and percentage uncertainty, an ellipsoid model to represent together angular and positional uncertainty, an ellipsoid envelope to show trajectory uncertainty and, a magic lens to expose additional properties in the lens areas and to select only objects satisfying certain uncertainty criteria. Li *et al.* [LFLH07] extend their previous work [LFH06, FH07] by adding uncertainty visualization to the presented astrophysical visualization tools. The algorithms presented processes 3D, static data and the main challenge is representing error and uncertainty.

Navrátil *et al.* [NJB07] describe visualizations used to examine a simulation of the formation of the first stars. Their visualizations capture the build-up and growth of bubbles of gas around the first stars which provides insight into the evolution of the early universe and guides future telescope observations. The authors use numerical simulation [SH02, SYW01], which involves 3D evolution of dark matter and gas coupled by gravity and radiation-hydrodynamics calculations, to study how the universe evolved from a simple homogeneous initial state through the formation of the first stars. The simulation produces particle data which is interpolated to the vertices of a regular grid using work by Jensen *et al.* [Jen96, JC98]. This interpolation method controls the number of particles used in the interpolation using both an inclusion distance for particles around the interpolation point and a maximum number of particles that are used in the interpolation. The resulting regular grid is imported into ParaView to extract isosurfaces and to smooth them. The authors use colour to differentiate between isosurfaces representing hydrogen density, molecular density and ionized molecules. They use transparency to show surface overlap. The isosurfaces show the build-up and growth of bubbles of either ionized gas or hot, heavy element-enriched gas. Simulation data

is 3D and time-dependent. The main challenge addressed by the paper is feature representation where the features are the gas bubbles represented using isosurfaces.

Fraedrich *et al.* [FSW09] explore scalability limitations in the visualization of large particle-based cosmological simulations and present techniques to work around limitations on current PC architectures. The authors address memory size and bandwidth limitations by using a multi-resolution hierarchy exploiting octrees, storing several tree nodes in a single disk page, culling particles that fall on the same pixel on the screen, discarding particles depending on their density contribution and using attribute compression. The authors use asynchronous I/O and pre-fetching to reduce disk access latency impact on performance. The authors use a vertex array buffer to store data on the GPU and a vertex shader to render the data. Particle data from a cosmological simulation is rendered in software by Dolag *et al.* [DRGI08]. Multi-resolution point splatting techniques are presented by Hopf and Ertl [HE03], Hopf *et al.* [HLE04] and Szalay *et al.* [SSL08]. The authors augment these techniques with out-of-core rendering and present an approach that is able to interactively visualize particle data exceeding 10 billion elements. Simulation data is 3D, static and the main challenge is scalable visualization.

4. Chemistry

Chemistry is concerned with the properties and structure of substances, the transformations they undergo and the energy exchanged during these processes. Physics studies the structure and behaviour of individual atoms whereas chemistry studies properties and reactions of molecules [bri10b].

See Valle [Val06] for a project that surveys chemistry visualization tools and methods and collects scientists' feedback on them. See Visualizing Chemistry [otNA06] for a review of the current state of the art in chemistry imaging techniques. This book has a concluding chapter with grand challenges and discussion of visualization and domain specific problems where the visualization community could help.

4.1. Nanotechnology

Nanotechnology is the manipulation of atoms, molecules and materials to form structures at nanometer scales. These structures typically have new properties differing from the building blocks due to quantum mechanics. Nanotechnology is an interdisciplinary field involving physics, chemistry, biology, material science and many engineering disciplines. The word nanotechnology refers to both the science and the engineering of the field [bri10e].

Included in our survey are contributions that visualize the formation of nanoparticles in turbulent flows [SIG05]*, and that present a web-based nanotechnology visualization tool [QMK*06].

Qiao *et al.* [QMK*06] describe the design and integration of a novel remote visualization framework into the nanoHUB.org, a science gateway for nanotechnology education and research. Users run simulations on super-computing resources and use remote hardware accelerated graphics for visualization from within a web browser. The authors created nanoVIS, a visualization engine library that can handle a variety of nanoscience visualizations involving vector flows and multi-variate scalar fields. This engine acts as the server end of the remote visualization and runs on a Linux cluster equipped with hardware acceleration. A VNC [RSFWH98] session uses the nanoVIS library to produce visualizations which are then transmitted over the Internet. The Rapid Application Infrastructure (Rappture) Toolkit [McL05] is used to generate the user interface for running a simulation and visualizing results. The nanoVIS visualization engine uses work by Qiao *et al.* [QEE*05] for visualization of multi-variate scalar fields using texture-based volume rendering and work by Kolb *et al.* [KLRS04] and Krüger *et al.* [KKKW05] for vector field visualization. The data that can be processed by the system is 3D, time-dependent, multi-variate scalar and vector data and the main challenge is scalable visualization.

4.2. Physical chemistry

Physical chemistry is concerned with measuring, correlating and explaining the quantitative aspects of chemical processes, rather than being focused on classes of materials that share common structural and chemical features. Modern physical chemistry does this using a quantum mechanical model of atomic and molecular structure [bri10b].

This section presents works focusing on visualizations of quantum chemistry simulations [QEE*05], [JV09]*.

Quantum dots (QDs) are nano-scale structures that can confine a small number of free electrons in a small space and allow control over the number of electrons and their excitation energy (i.e. material properties). This leads to promising applications such as infrared detectors, lasers with tunable wave-lengths, high-density low energy consumption memory chips, and logical gates for quantum computing. Qiao *et al.* [QEE*05] describe a method and system for visualizing data from quantum dot simulations (QDs) which is in the form of two Face-Centred Cubic lattices (FCC). The described hardware-accelerated volume rendering approach and application (Figure 3) allows scientists to interactively visualize, navigate and query QD simulations.

Decomposing the FCC lattice can result in an enormous number of tetrahedra, which makes rendering multi-million atom simulations difficult. The authors achieve interactivity by using a 3D texturing approach with a logarithmic transfer function. The software can also render multiple fields at once, and perform simple GPU statistical calculations on the selected data through the use of fragment shaders to obtain

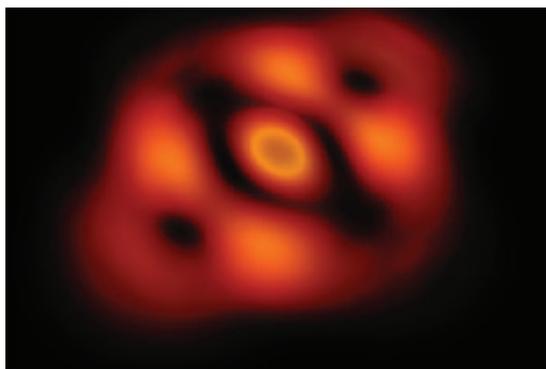


Figure 3: The electron orbitals of a Indium-Arsenide Quantum Dot device in the third excited state, showing S and s^* orbitals with up and down spins [QEE*05]. Image courtesy of David Ebert.

a) the number or percentage of orbitals satisfying one or more criteria and b) the percentage contribution of orbitals to the total electron cloud. It builds on the approach of Rober *et al.* [RHEM03] for BCC (body-Centred cubic) grids and Westerman and Ertl's work on 3D texturing [WE98], and performs queries using the techniques of Buck *et al.* [BFH*04] and Krüger and Westermann [KW05]. The dimensionality of the data is 3D, static, multi-attribute, uniform resolution on a non-cartesian lattice and the main challenge is using the GPU for volume rendering multi-variate wave functions.

4.3. Organic chemistry

Organic chemistry studies the correlation between the physical and chemical properties of substances with their structural features. This has great applicability to the design and synthesis of novel molecules with some desired properties. Most visualization for organic chemistry show the 3D structure of molecules [bri10b].

We survey papers that visualize molecules [BDST04, TCM06], molecular surfaces [CS04, CS05, KBE09, LBPH10], paths of molecules to possible binding sites [LBH11], visualize and track protein cavities [KFR*11] and the solvent pathlines near them [BGB*08]*, detect anomalous structures in molecular dynamics simulation data [MHM*04], determine states of energy minima and represents relationship between these states in a chemical system [BWH*11].

Transformation in chemical systems can be studied by considering its energy as a function of the coordinates of the system's components. These energy functions are high-dimensional and chemists lack effective visualization techniques to handle them. Beketayev *et al.* [BWH*11] develop a new technique that enables this analysis. The system combines concepts from topological analysis, multi-dimensional scaling and graph layout to produce a visualization of the

energy function that focuses on the energy minima (stable states) of the system and their relationships to each other. The closest related work is that of Flamm *et al.* [FHSS07] and Okushima *et al.* [ONIS09] on topological analysis in chemistry, and that of Gerber *et al.* [GBPW10] on visual analysis for chemistry. Simulation data is 3D, time-dependent, uniform and the main challenge is feature detection where the features are states of energy minima and the relationships between these states.

Bajaj *et al.* [BDST04] describe both an application that uses the GPU to accelerate 3D image-based rendering of molecular structures at varying levels of detail, and an alternative approach to interactive molecular exploration using both volumetric and structural rendering together to discover molecular properties. Their approach results in an order of magnitude speedup over traditional triangle based rendering and enables visualization of large and previously intractable molecules. Using NVIDIA's Cg, the authors extend impostor rendering from spheres to cylinders and helices in their TexMol application. They also implement volumetric visualization using 3D texture mapping, and enable multiple views (structural and volumetric) to be displayed and linked together. Their use of graphics hardware allows the rendering to approach interactive frame-rates. The structural renderer used in this work was described previously in The Cg Tutorial [FK03]. The view-dependent texture mapping techniques are described in work by Debevec *et al.* [DYB98]. The phenomena being studied is 3D, static and the main challenge is using graphics hardware for rendering regular curved surfaces encountered in molecular visualization.

Mehta *et al.* [MHM*04] seek to detect anomalous (non-ideal) structures in silicon substances. They propose a method to automatically generate a salient iso-value that can discriminate the anomalous structures. This is used to generate both a surface visualization and volume rendering of the data. The salient iso-surface is obtained by (i) generating a histogram of the electron density scalar field, (ii) smoothing the histogram using a Gaussian kernel, (iii) applying FFT, (iv) convolving with a band-pass filter to amplify the high frequency component and (v) applying an inverse Fourier transform to obtain the enhanced histogram. The histogram bins where the curvature of the histogram is large are taken as the salient values. These values are averaged to obtain the salient iso-value which is used to generate both an isosurface and volume rendering of the data. The anomaly detection can be achieved through data processing techniques alone such as through common neighbour analysis (CNA) [CJ93] or solely visualization [VBJM*95]. This paper uses a mixture of the two. Simulation data is 3D, static, uniform resolution, regular grid and scalar data and the main challenge is feature detection where the features of interest are anomalous structures in silicon substances.

Cheng *et al.* [CS04] present a new skin model of molecules that are calculated directly from a van der Waals force model.

The challenge is to create skin mesh models that are of good quality, provably correct, fast to compute and algorithmically convergent. Their approach is to use an advancing front surface method that constructs a Restricted Delaunay Triangulation over the model surfaces. However, when advancing triangles, sometimes they may overlap which causes robustness problems. They overcome this challenge through computing a Morse–Smale complex to simplify the topological changes. Further, to achieve a homeomorphic mesh with high quality they reduce the size of the triangles to be proportional to the radius of the maximum principle curvature of the surface. The Marching Cubes algorithm [LC87] can achieve topological surfaces at high speed but the surface elements are not necessarily homeomorphic to the original surface. Similar to this work, Stander *et al.* [SH05] track the critical points of the implicit function by Morse Theory and Amenta *et al.* [ACDL00] generate a homeomorphic mesh, but each method can create bad shape triangles having extreme sharp or obtuse angles. Data processed is 3D, static, uniform resolution—but the size of triangles is determined by the curvature, no explicit grid and scalar data. The main focus of the paper is mesh generation for a new skin model of molecules.

Cheng *et al.* [CS05] present a surface triangulation algorithm that generates a mesh for the molecular skin model [Ede99]. This is the first robust algorithm that is capable of generating a mesh with guaranteed lower bound on the minimum angle of each triangle in the surface mesh. The authors employ a Delaunay-based method to generate a mesh for the molecular skin model incrementally. They add one sample point each time and maintain the Delaunay triangulation of the sample points with the incremental flipping algorithm [Law77]. They extract a subset of the Delaunay triangulation as a candidate surface triangles. These candidate surface triangles guide the future point sampling. This procedure is applied iteratively until it obtains a ϵ -sampling of the molecular skin surface. This algorithm provides better efficiency than work by Cheng *et al.* [CDES01] and more robustness than work by Cheng and Shi [CS04]. The algorithms presented handle 3D, static data and the main challenge is generating a mesh for a molecular surface model.

Tarini *et al.* [TCM06] present a set of techniques to enhance the real-time visualization of molecules using the space-fill and the balls-and-sticks approaches. These techniques enhance the user's understanding of the 3D shape of molecules while they maintain real-time rendering speed. Tarini *et al.* use impostors to render the two types of primitives in molecule visualization: spheres and cylinders. The impostors are procedural, which means that all geometric attributes are synthesized in the GPU. The authors integrate additional ways of enhancing the images' visual quality including depth aware contour lines as in work by Deussen *et al.* [DS00] and halo effects as in work by Luft *et al.* [LCD06]. Tarini *et al.* implement ambient occlusion [Lan02] using a similar approach with work by Sarletu *et al.* [SK04]

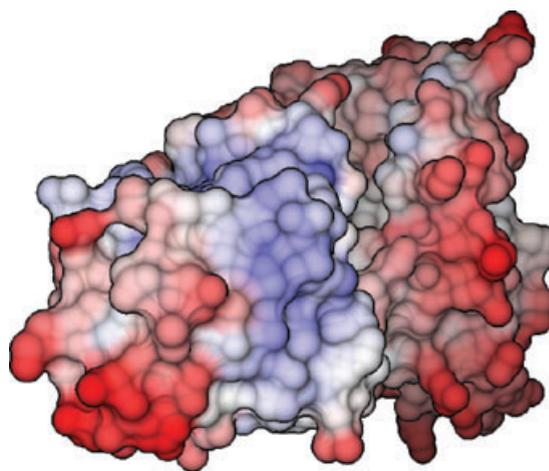


Figure 4: Solvent excluded surface coloured according to the temperature factor of the protein. [KBE09]. Image courtesy of Thomas Ertl.

and by Pharr [PG04]. The techniques described handle 3D, static, unstructured grid data. The main challenge is using the GPU to maintain real-time rendering speed while enhancing the user's understanding of the 3D shape of large molecules.

Krone *et al.* [KBE09] present an approach for visualizing the solvent excluded surface (SES) of proteins using a GPU ray-casting technique. They achieve interactive frame rates even for long protein trajectories and thus enable analysis of time-dependent molecular simulations (Figure 4). The surface of molecules is important for studying protein-protein or protein-ligand interactions or for exploration of phenomena which occur at the surface, such as binding sites or hydrophobic and hydrophilic regions.

The ReducedSurface (RS) [SOS98] is used to render the SES because it can be computed fast and it can be efficiently updated piecewise between two consecutive timesteps. Krone *et al.* [KBE09] use acceleration techniques to achieve interactive frame rates for rendering long trajectories. First, they filter out unwanted protein motion [Kab76] and second they reduce the raw atomic data [BHI*07]. The authors use several visualization techniques for enhanced protein analysis: utilize various standard colouring schemes, enable better depth perception using linear distance fog or depth darkening [LCD06] and enable better perception of shape using depth dependent silhouettes. Connolly [Con83] presents the equations to compute SES analytically. Sanner *et al.* [SOS98] develops the Reduced Surface which accelerates the computation of SES. Chavent *et al.* [CLM08] present a related visualization application of a GPU ray-casting of the Molecular Skin Surface. This works improves on available molecular viewers in two ways. First it requires less memory because it uses GPU ray-casting as opposed

to polygon based rendering. Second, it dynamically updates the SES and thus it enables analysis of arbitrary large molecular simulation trajectories. The algorithms presented process 3D, time-dependent, scalar, unstructured, multi-attribute data. The main challenge is utilizing the GPU to raycast the implicit mathematical description of the SES.

Lindow *et al.* [LBPH10] present ways to accelerate the construction and the rendering of the solvent excluded surface (SES) and the molecular skin surface (MSS) which are used in visualizing the dynamic behaviour of molecules. This is important to domain scientists as the function of a biomolecule is driven to a large extent by its 3D shape. The authors propose using the contour-buildup algorithm [TA96] for building SES because it is easy and efficient to parallelize. They adapt the approximate Voronoi diagram algorithm [VBW94] for computing MSS. This algorithm was originally used to compute SES. Molecule surfaces are directly visualized on the GPU similarly to Krone *et al.* [KBE09] and Chavent *et al.* [CLM08]. The main reason for improvements in the rendering of the SES surface is the use of tight-fitting bounding quadrangles as rasterization primitives. Improvements in MSS rendering speed are caused by using tight-fitting bounding quadrangles for the convex spherical patches, using 3D polyhedra instead of mixed cells of MetaMol [CLM08] and removing empty mixed cells already on the CPU. The authors accelerate the constructions and rendering of SES and MSS which improves on work by Krone *et al.* [KBE09] and Chavent *et al.* [CLM08], respectively. The results are demonstrated on 3D, time-dependent data. The main challenge is efficiently utilizing the GPU to raycast the algebraic surfaces that compose SES and MSS.

Lindow *et al.* [LBH11] focus on the challenge of computing and visualizing molecular binding sites and paths leading to these sites. These paths can help in understanding molecular interactions which is key to answering many open questions in biochemistry and biology. As part of their interactive visualization, advanced shading, rendering and lighting methods are utilized to make features of interest, such as deeply embedded paths, more visible and prominent to the user. The paths are computed based on a Voronoi diagram of spheres from the van der Waals spheres for the molecule. The significant paths are determined by filtering the topology graph from the Voronoi diagram based on five factors: radius, regular branches, edges, cycles and duplicate branches. The user is then able to select particular paths of interest and explore the molecule with the interactive visualization. In computing the Voronoi diagram, the authors used the method of Gavrilova *et al.* [GR03]. For edge tracing in the Voronoi diagram of spheres, the authors used methods from Kim *et al.* [KCK05] with further techniques from Cho *et al.* [CKL*06]. The methods presented process 3D, static, scalar, unstructured, multi-attribute data. The main challenge is feature detection where the features are the paths of molecules to possible binding sites.

Krone *et al.* [KFR*11] present a method for interactive extraction and tracking of cavities within time-varying protein data. In molecular dynamics, identifying cavities in proteins in substrates is important: these cavities can often be found close to the active centre of the protein. If the cavities open up to the environment by reaching the surface of the protein, then the active site is made accessible to the surrounding substrate which is essential for certain reactions. Existing tools only work for static snapshots and do not operate in real-time which means they do not allow the exploration of time-dependent structural changes. A steerable visualization interface is provided: the simulation data is shown in 3D, and cavities can be selected and tracked via a 2D slice. For the 3D view, the authors use an SPH-like technique to obtain a continuous density volume which is visualized by ray-casting. A Region Growing algorithm computes the cavity size which is then shown graphically on screen. Existing tools dealing with this type of data include CAVER[POB*06], PocketPicker[WPS*07] and MOLE[PKKO07]. The presented methods work on 3D, time-dependent scalar, unstructured grid. The main challenge is protein cavities detection and tracking.

5. Earth Sciences

We take Earth Sciences to include geology, hydrology and atmospheric sciences [bri10d]. It includes the study of water, both underground, in rivers and oceans, and in ice-caps and glaciers; of phenomena associated with the atmosphere and climate; and of the physical and chemical structure of the earth and its history.

5.1. Atmospheric sciences

Atmospheric sciences deal with the properties, structure and composition of the atmosphere, understanding atmospheric phenomena such as clouds, fog and dew, and understanding and predicting the weather.

We present research to visualize storm and cloud-scale simulation data [REHL03]*, to visualize warm rain formation and compare weather models with radar observation [SYS*06]*, to analyse air pollution [QCX*07], to visualize the uncertainty associated with weather prediction[SZD*10]*, and to simulate and visualize cyclones[MNV10].

Qu *et al.* [QCX*07] present weather data visualization to analyse air pollution in Hong Kong. They visualize attributes describing air quality and they allow the exploration of correlations between these attributes. Wind speed and direction are the primary attributes driving the exploration of other attributes that describe air quality, such as concentration of various chemicals in the air. Qu *et al.* [QCX*07] use a polar coordinate system to show the correlation of an attribute with wind speed and direction, with the values of the attributes shown using a colour map. A sector of interest can be selected from the polar coordinate display. A pixel bar chart [KHD02]

is shown that depicts three additional attributes (axes X, Y and colour) for a certain wind direction and speed. Data can be explored using parallel coordinates [ID90]. A correlation coefficient [QCX*07] detects linear dependencies between attributes for normally distributed data and a weighted complete graph is used to show this correlation. Work by Barnes and Hut [BH86] and Noack [Noa05] is used to draw a graph in which the distance between nodes reflects the strength of the correlation. The correlation is also encoded in the width of the edges of the graph. The weighted complete graph can be used to reorder the axes of the parallel coordinates visualization such that highly correlated attributes are close together. This paper uses and adapts standard techniques such as polar coordinates, colour-mapping, parallel coordinates and pixel bar charts to visualizing air quality measures in Hong Kong and exploring their correlation. The phenomena being studied is 2D, time-dependent, scalar, multi-attribute on a unstructured grid. The main challenge addressed by the paper is multi-field visualization.

Malakar *et al.* [MNV10] present an adaptive framework that performs cyclone simulations and remote online visualization as part of a system in which the frequency of the output from the simulation is adjusted based on application and resource dynamics. The goal is to enable continuous progress in the simulation and to maximize temporal resolution in visualization, taking into account limitations in storage and network capacities. The implementation uses a software layer to determine the number of processors to be used for simulation and the frequency of output of climate data based on the network bandwidth, the free disk space and the resolution of the climate simulation. The authors describe two algorithms for processor allocation: a greedy algorithm that tries to maximize the simulation rate and an optimization-based approach that attempts to provide a steady-state simulation and visualization rate. The greedy algorithm makes decisions to reduce or increase the number of simulation processors for free disk space equal to 10%, 25% and 50% of the total disk space. The optimization-based approach uses linear programming to determine the number of processors for simulation and the frequency for output. Two solutions have previously been proposed for online visualization of numerical simulations—i.e. performing the visualization at the same time as the simulation so as to avoid storing the simulation output for all the time steps. First, there is a tightly coupled execution of the simulation and visualization components [TYRG*06, MWYT07, Ma09], where simulation is followed by visualization on the same set of processors. The drawback here is that the simulation component is generally more compute-intensive than the visualization, which means that visualization results are produced after a considerable delay. A second solution [EGH*06] uses shared memory for communication between simulation and visualization which requires a large amount of shared memory to service both sets of demands. Weather simulation data is 2D and time-dependent with adaptive-resolution. The main challenge is scalable visualization.

5.2. Climatology

Climatology[bri10c] is concerned with climate differences between different regions and climate changes over long periods of time. Climatologists seek to identify slow-acting influences on weather and to identify the consequences of climate change.

We review papers that visualize climate variability changes [JBMS09]*, identify regions in the atmosphere that act as indicators for climate change [KLM*08], describe visualization for public-resource climate modelling [SFW04*] and perform time-lag analysis and drought assessment on satellite observational data [KGH*09].

Kehrer *et al.* [KLM*08] use visualization and interaction technologies to identify regions in the atmosphere that can act as indicators for climate change. These regions are subsequently evaluated statistically. Multiple linked views allow the exploration and analysis of different aspects of multi-field data. A synthesized *degree-of-interest* (DOI) attribute can be used to specify a data region in focus. Smooth brushing (fractional DOI values) and logical combination of brushes are supported. This work uses and extends the SimVis [DGH03, DH02, DMG*04, MKO*08] framework for climate research. Extensions to SimVis include: four-level focus and context visualization, a function graphs view, data aggregations and image space methods for maintaining responsiveness when interacting with the data, and enhanced brushing techniques to deal with the temporal nature of the data. The dimensionality of the data is 3D, time dependent, multi-attribute scalar on a structured grid. The main challenge is feature detection, where the features are areas that can act as indicators for climate change.

Kendal *et al.* [KGH*09] integrate techniques in parallel I/O with concepts from parallel query-driven visualization. The driving application is to study over a terabyte of multi-variate satellite data for drought assessment (Figure 5) and time-lag analysis. They reduce the end-to-end execution times on these problems to one minute on a Jaguar Cray XT4.

The authors use their system to discover climatic trends based on a vegetation index, a water index and a drought index. They use five criteria to find periods of drought: water index below a threshold, vegetation index below a threshold, drought index in a certain range, a minimum time span and a maximum number of years of drought. They visualize the time-lag between the first snow fall and the first sign of green-up from vegetation. They first query the vegetation and water indexes on certain ranges and then parallel-sort the results in the spatial and temporal domains. The authors use collective I/O [TGL99] to achieve better bandwidth rates in the I/O phase, a query-driven method [GMHG06] for scalable contour extraction and visualization, and the parallel sample sort [BLM*98] for performing temporal analysis. Satellite data is 2D, time-dependent on a regular grid. The main challenge is scalable visualization.

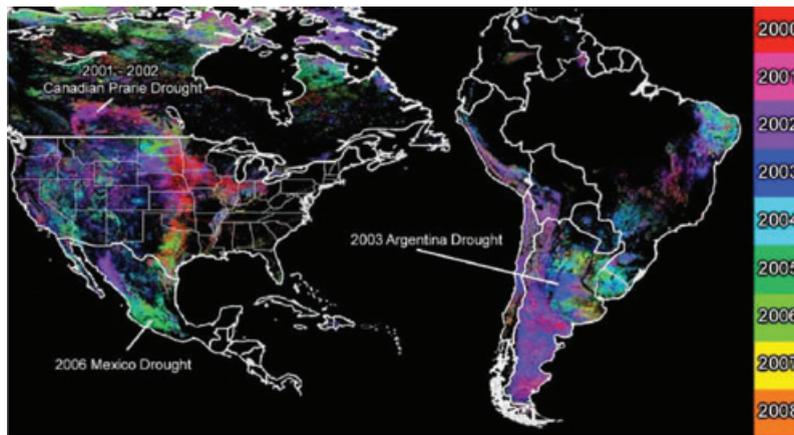


Figure 5: Periods of drought that lasted for at least 2 months and occurred for up to 2 years for any given region [KGH*09]. Image courtesy of Jian Huang.

5.3. Hydrology

Hydrology concerns the waters of the Earth, their distribution and circulation, and their chemical and physical properties.

We present a study of visualization tools for an environmental observation and forecasting system for the Columbia River [JCSB03], a paper that focuses on detection and visualization of mesoscale eddies in an ocean simulation [WHP*11], and work that visualizes changes in the frontal position of marine-terminating glaciers in Greenland [DBS*11]

Drocourt *et al.* [DBS*11] present a design study on visualizing spatiotemporal data of changes in the frontal position of marine-terminating glaciers in Greenland, resulting in a family of radial visualizations. The scientists are interested in the movement of these glaciers, in light of a changing climate, as they contribute directly to sea level rise by releasing icebergs into the ocean. The authors developed an automated algorithm to partition the visualization into quadrants based on a certain number of key glaciers. The distribution in each quadrant is then relaxed to spread the radial points out further. Other examples of time-series visualization include Havre *et al.*'s Themeriver [HHWN02]. This work also provides a solution to some of the issues raised by Borgo *et al.* [BPC*10] regarding inaccuracy in change evaluation based on pixel-based visualization. Studied phenomena are 2D, time-dependent, multi-field, point data. The main challenge is time-dependent visualization.

Ocean simulations produce high-resolution, 3D data fields, but publications in oceanography typically show 2D plots of variables in horizontal or vertical sections. Williams *et al.* [WHP*11] visualize and analyse flow data from a 3D ocean simulation with a particular focus on coherent vortical features called mesoscale eddies. These eddies represent a large fraction of the total estimate of oceanic kinetic

energy; they have a significant influence on the earth's climate by transporting heat, momentum and mass; and they are important to the biology of the oceans as they transport carbon, oxygen and nutrients to nutrient-poor waters. Eddies are identified by first calculating the value of the Okubo-Weiss parameter at each point in the simulation. The algorithm then selects only those areas in which this parameter indicates that vorticity dominates and the flow is circular in nature. Finally, the eddy field is shown in 3D with eddies depicted as cylinders, with colour-mapped to rotation direction and spatial extent corresponding to that of the eddy. This paper is similar to other work on extracting structure and visualizing it through glyphs [TG09], and previous work on visualization of vortices in 3D [ZM95]. The dimensionality of the data is 3D, static, uniform resolution data on a regular grid. The main challenge is feature detection, where features of interest are coherent vortical areas called mesoscale eddies.

Jimenez *et al.* [JCSB03] present visualization tools for an environmental observation and forecasting system for the Columbia River [JCSB03] (CORIE). The authors add interactive 3D visualization tools to CORIE which can be used to inspect the simulated and measured data. The Columbia River is the target of numerous studies focusing on life cycles of endangered fish species in the context of navigation and hydropower improvements and ecosystem re-saturation efforts. A key challenge is to separate natural from man-made effects. The work uses VTK to add three-dimensional surface and volumetric visualization capabilities to the CORIE (environmental observation and forecasting) system. A custom volume renderer is used with the VTK code. The work uses an unstructured volume rendering engine similar to that of Lum *et al.* [LMC02]. The visualization techniques presented process 3D, time-dependent, unstructured grid, scalar and vector data. The main challenge is multi-field visualization, where data of interest includes bathymetry, salinity scalars, velocity fields and drifters for the CORIE system.

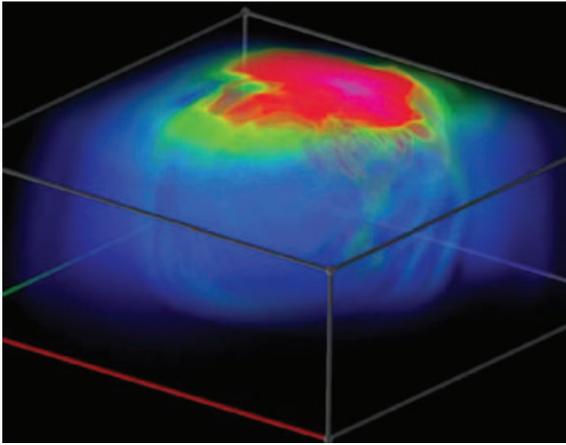


Figure 6: Earthquake simulation. Image shows the ground motion after the seismic waves have hit the surface [MSB*03]. Image courtesy of Jacobo Bielak.

5.4. Geology

Geology is the scientific study of the Earth, its composition, structure and physical properties.

Included in our survey are contributions that visualize hot fluid discharges from seafloor vents [SBS*04]*, produce illustrative rendering of geologic layers [PGTG07], visualize seismic data together with satellite-based observational data [YXG*10]*, and present scalable visualizations of large-scale earthquake simulations [MSB*03, YMW04, TYRG*06].

See Carr [Car02] for a book on data visualization techniques for geosciences and Erlebacher *et al.* [EYD01] for a review article on geoscience visualization techniques, and areas that need improvement.

Ma *et al.* [MSB*03] present a parallel volume visualization algorithm for interactive rendering of time-varying, unstructured data generated from large-scale earthquake simulations (Figure 6). High-resolution exploration of the data was not available in the past to geoscientists who were instead limited to visualizations of reduced-resolution versions of the data on a regular grid.

The rendering algorithm uses a spatial (octree) encoding of the data for adaptive rendering. The appropriate octree level is selected based on the image resolution. A host computes the octree and uses it to distribute blocks of hexahedral elements among rendering processors. The centralized data distribution is not ideal as parallel I/O should have been used instead. Each processor executes a ray-casting and an image compositing operation while the data block for the next time-step is transferred from disk. The authors use SLIC [SML*03]

for image compositing. The data is 3D, time-dependent on an unstructured grid, and the main challenge is scalable visualization.

Yu *et al.* [YMW04] present a parallel visualization pipeline to study an earthquake simulation that models the 3D seismic wave propagation of the 1994 Northridge earthquake. Their tests show that they completely remove the I/O bottleneck, common in time-varying data, caused by the need to constantly transfer each time step from disk to memory. However, optimizing access to storage remains an important challenge for visual analysis of large datasets [RPS*08]. The authors use parallel I/O strategies that adapt to the data size and parallel system performance. The visualization pipeline includes input, rendering and output processors. The input processors read data files from the parallel file system, pre-process the raw data, and distribute the resulting data blocks to the rendering processors. The rendering processors produce volume-rendered images for its data blocks which are then delivered to the output processors and finally to a display. The authors extend previous work [MSB*03] by improving the I/O scheme. This allows them to reduce I/O and pre-processing times down to rendering time, making possible to reduce these costs by overlapping I/O and rendering. The authors visualize 3D, time-dependent data on an unstructured grid. The main challenge is scalable visualization, specifically on working around the problems of large-scale I/O.

Tu *et al.* [TYRG*06] describe an end-to-end approach to a simulation pipeline in which all elements (problem description, solver and visualization) are tightly coupled and execute in parallel with no intermediate I/O. They use this new approach for an octree-based finite element simulation of earthquake ground motion. Performance evaluations demonstrate that the end-to-end approach overcomes the scalability bottlenecks of traditional approaches. The key idea used by the authors is to replace the traditional file interface with a scalable, parallel runtime implemented on top of a parallel octree data structure. All components of the simulation pipeline (meshing, partitioning, simulation and visualization) are tightly coupled and execute on the same set of processors. The inputs are the simulation and visualization specifications whereas the outputs are image frames generated as the simulation runs. There is no other file I/O. The authors use an octree-based earthquake modelling method [BGK05], a database system to generate unstructured hexahedral octree-based meshes [TO04] and, scalable rendering calculations [MSB*03, YMW04]. The earthquake simulation data is 3D, and time-dependent on an unstructured grid. The main challenge is scalable visualization.

Patel *et al.* [PGT*08] present a toolbox for interpretation and automatic illustration of 2D slices of seismic volumetric reflection data. They improve both the manual search and the annotation of seismic structures, reducing the manual labour of seismic illustrators and interpreters (Figure 7).

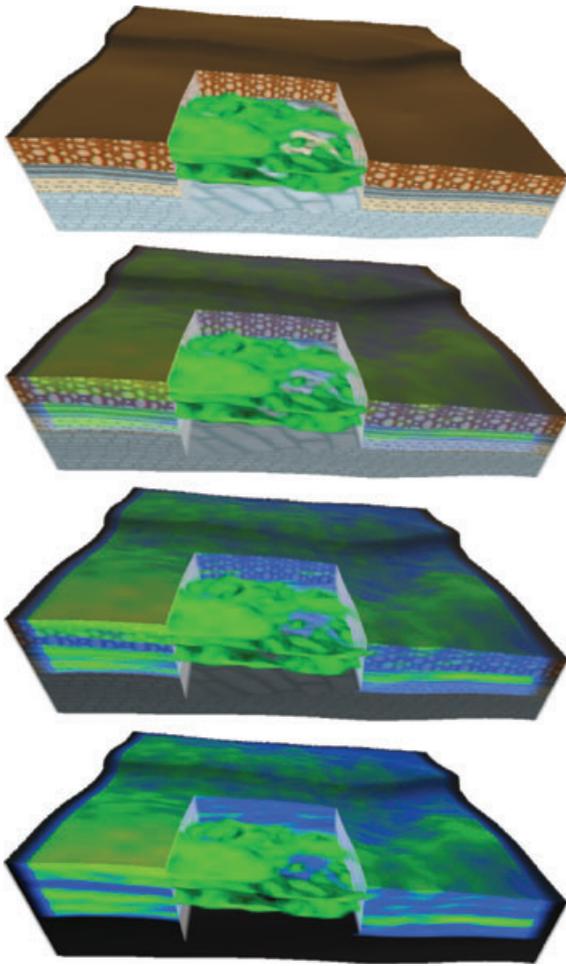


Figure 7: Blending from illustrative rendering (top) to uninterpreted data rendering (bottom) for seismic volumetric reflection data. [PGTG07]. Image courtesy of Daniel Patel.

The authors improve the search of seismic structures by pre-calculating the horizon lines that separate rocks with different mineral densities or porosity characteristics. They improve the illustration of seismic data by using deformed texturing and line and texture transfer functions. The authors extend their previous work [PGTG07] by automatically interpreting horizon lines and by providing transfer functions for lines, wells and horizon lines. Seismic data is 3D, static, scalar attributes on a structured grid with uniform resolution. The main challenge of the paper is feature detection, where the features are the lines that separate rocks with different mineral densities or porosity characteristics.

6. Physics

Physics studies the structure of matter and the interactions between objects at microscopic, human and extragalactic

scales. It is the synthesis of several fields including mechanics, optics, acoustics, electricity, magnetism, heat and the physical properties of matter. This synthesis is based on the fact that the forces and energies studied in these sciences are related [bri10g].

6.1. Acoustics

Acoustics is the science of sound, its production, transmission and effects. Acoustics studies phenomena responsible for the sensation of hearing, sounds with frequency too high or too low for the human ear, and the transmission of sound through media other than air [Pie89].

We review papers that simulate sound within a room [BDM*05, LCM07b, CLT*08, BMD*08], that show how the material on room surfaces influences sound [DMB*06, MDHB*07], and present a comparative visualization of two different approaches for acoustic simulation [DBM*06].

Bertram *et al.* [BDM*05] trace the paths of phonons (sound particles) from a sound source in a scene to a listener's position. This enables the computation of a finite-response filter that, when convolved with an anechoic input signal, produces a realistic aural impression of the simulated room. The results from this technique are more precise than those from finite element simulations for higher frequencies. The implementation is similar to that of photon mapping: particles are followed from source and through reflections (using material-specific properties). Bidirectional reflection distribution functions (BRDF) are used to determine local intensity. The technique of photon mapping [Jen96, JC98, KW00] was an inspiration for this work. Previous work in acoustics is divided into image-source [Bor84], accurate but complicated for non-box shaped rooms, and ray tracing [Kul85], which is computationally expensive and receiver-location dependent. Processed data is 3D and time-dependent. The main challenge addressed is performing the sound simulation.

Deines *et al.* [DMB*06] present visualizations of acoustic behaviour inside a room. Through these visualizations the authors show the surface material's influence on the sound coming from the source, the energy of the sound reflected by various surfaces at different time intervals, and a global view of the received sound at listeners' positions (Figure 8).

The authors present four visualization techniques for acoustic behaviour. They visualize phonons on surfaces by rendering each phonon as a sphere and colour-coding it according to its spectral energy. A second technique visualizes wave fronts reflected at the room surfaces by clustering phonons with a common history and colour-coding the resulting surface based on the energy of the phonons. The phonon clusters reduce to a simple phonon as the number of reflections increases, so this technique works only for visualizing wave fronts of phonons resulting from a few reflections. A

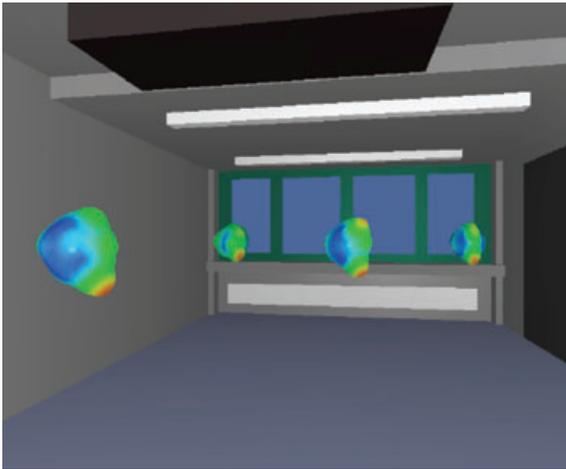


Figure 8: *Acoustic behaviour inside a room [DMB*06]. Spheres at four listener positions which are deformed by the overall energy spectrum and colour-coded by the energy at 80 Hz. Most energy at 80 Hz is reflected at the floor and at the ceiling. Image courtesy of Eduard Deines.*

third technique produces a continuous representation of the emitted energy on the surfaces of the room by interpolating the energy and pathlength of the phonons. Finally, a fourth technique shows a deformed sphere according to the amount of energy received from various directions, colour-coded based on the frequency of the sound received. Deines *et al.* [DMB*06] use their previous acoustic simulation algorithm [BDM*05] to visualize acoustic room properties and the sound properties at the listener position. Sound simulation data is 3D, time-dependent, scalar and vector attributes, on an unstructured grid. The main challenge is multi-field visualization showing both the energy and the frequencies of phonons at listener positions.

Deines *et al.* [DBM*06] present a comparative visualization of two different approaches for acoustic simulation: a finite element (FEM) based solution of the sound wave equation (precise, but computationally expensive at medium and high frequencies) and phonon tracing (efficient but not precise at low frequencies). The goal of this work is to learn in which range of frequency the results of both methods match and to devise a measure of the differences between the two methods. Phonon tracing [BDM*05] fails in the low frequency range because of diffraction and interference effects, so wave acoustics is used to simulate the low frequency part of the sound field. As an alternative, the authors use the FEM to solve the wave equation. This method approximates the wave equation by a large system of ordinary differential equations the solutions of which are the pressure at grid points covering the room. Deines *et al.* [DBM*06] devise a simulation experiment to compare the two approaches by using

an acoustic measure called gain and displaying the resulting error. Furthermore they visualize the interference patterns and wave propagation for different frequencies of the signal. Through these visualizations, they are able to conclude at which frequency range the two methods match. The authors extend their previous acoustic simulation method phonon tracing [BDM*05] by using pressure instead of energy in simulation calculations. The phenomena they study is 3D, time dependent, on an unstructured grid. The main challenge is doing comparative visualization to aid in studying alternative methods for acoustic simulation.

Lauterbach *et al.* [LCM07b] present a new algorithm for interactive sound rendering that can handle complex scenes with tens or hundreds of thousands of triangles, dynamic sound sources and dynamic objects. The authors follow sound through a scene through *frustum tracing* by handling direct transmission or specular reflection. They trace a convex frustum through a bounding volume hierarchy that represents the scene. The frustum is defined by the four side facets and the front face. The main difference between frustum tracing and beam tracing is how the intersection with a scene triangle is calculated. Beam tracing calculates the exact intersection. In frustum tracing, the frustum is subdivided uniformly into smaller sub-frusta and only discrete clipping is performed at the sub-frusta level. Lauterbach *et al.* [LCM07b]'s algorithm can be thought of as a discrete version of the beam tracing algorithm by Funkhouser *et al.* [FCE*98, FTC*04]. Frustum tracing is faster but less precise compared with beam tracing. Precision can be improved through finer sub-division into smaller frusta at the cost of speed. The techniques described handle 3D, time-dependent, multi-attribute scalar data on an unstructured grid. The main challenge is computing the acoustic simulation.

Chandak *et al.* [CLT*08] present an interactive algorithm that computes sound propagation paths in complex scenes and can be used in acoustic modelling, multi-sensory visualization and training. Their algorithm can offer considerable speed-up over prior geometric sound propagation methods. The authors trace sound propagation paths for specular reflection and edge diffraction by tracing an adaptive frustum from a point source to the listener. The adaptive frustum is represented using an apex and a quadtree to keep track of its subdivision. The scene is represented using a bounding volume hierarchy of axis-aligned bounding boxes. The frustum is automatically sub-divided to accurately compute intersections with the scene primitives up to a maximum-subdivision depth. Chandak *et al.* [CLT*08] improve on the ray-frustum approach in Lauterbach *et al.* [LCM07a, LCM07b] by adaptively subdividing the ray-frustum in places where the scene has more complexity and adding edge diffraction to their sound modelling. Sound data is 3D, time-dependent, multi-attribute scalar, on an unstructured grid and the main challenge of the paper is using the science of sound to do the sound simulation.

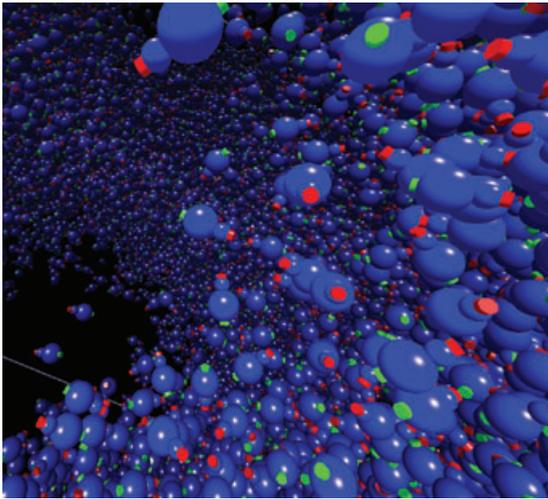


Figure 9: Synthetic dataset consisting of dipoles, visualized with depth cues turned on [RE05]. Image courtesy of Thomas Ertl.

6.2. Atomic, chemical and nuclear physics

We now turn to studies of matter at the smallest scale at which chemical elements can be identified and even at the structure of atomic nuclei. The most important properties of matter that we encounter in normal experience depend only on the mass of the atomic nucleus and its charge [bri10g, col07].

This section reviews research that visualizes particle data generated by accelerator modelling simulations [CFG*05]*[RPW*08], defects in nematic liquid crystals [SPL*06]* [MJK06] and nematic liquid crystal alignment [JKM06] and visualize large molecular dynamics simulations [RE05, GRDE10]. We review a paper that visualizes Fourier transform mass spectrometry experiments [BvL06]*, and a hardware accelerated simulation of radiographs applied to the simulation of experimental diagnostics for fusion experiments [LCM*05].

Reina *et al.* [RE05] describe a method for visualizing molecular dynamic simulations using the GPU that minimizes the quantity of data that needs to be transferred by generating implicit surfaces directly in the fragment program. This approach allows domain experts to visualize the results of simulations with a higher number of particles than before and offers better visual quality (Figure 9).

An existing pointcloud renderer is extended by writing fragment programs to ray-trace an implicit surface for each point in the data, which can contain multiple attributes. This work builds on the existing algorithm and renderer introduced by Hopf and Ertl [HE03] and developed further in work by Hopf *et al.* [HLE04] The method described handles 3D, time-dependent, adaptive resolution data. The main challenge is

efficiently using the GPU to ray trace implicit surfaces used to represent molecules.

Rübel *et al.* [RPW*08] combine infovis and scientific data management techniques to gain insights from a large, multi-field dataset produced by a laser wakefield accelerator simulation (Figure 10). These accelerators are of interest because they are able to achieve very high particle speeds within a relatively short distance when compared with traditional electromagnetic accelerators. Their approach performs particle tracking in a few seconds compared with hours when using a naive script.

The authors adapt and extend histogram-based parallel coordinates for use with high-performance query-driven visualization of very large data (210 GB). Parallel coordinates are used for both visual display and interactive construction of boolean data range queries. The queries are used for subsequent data mining operations. Index/query technology is used to mine for data and to generate multi-resolution histograms. Views of the data include a parallel coordinates view showing all particles, a 2D plot of the beam of highly accelerated particles and a volume rendering of the plasma density waves generated inside the accelerator. Rübel *et al.* [RPW*08] build on the parallel coordinates work of Novotny and Houser [NH06] to make it parallel and scalable to large data. They use the query-driven visualization work of Stockinger *et al.* [SSWB05], FastBit[fas]: software for bitmap indexing, and VisIt[vis]: software for data processing and visualization that can handle extremely large datasets. Data visualized is 3D, time-dependent, multi-field, particle data. The main challenge addressed by the paper is scalable visualization.

Liquid crystals are an intermediate phase of matter between solid and liquid. In this state, molecules do not favour any particular position but they do favour alignment with preferred directions throughout the material. Nematic liquid crystals (NLC) are a class of liquid crystals with elongated molecules. A common way to represent the average alignment of molecules within this type of material is the alignment tensor. Jankun–Kelly and Mehta [JKM06] introduce a glyph-based method for visualizing the nematic liquid crystal alignment tensor. Their method communicates both the strength of the uniaxial alignment and the amount of biaxiality and, unlike previous methods, does not distort features of interest. Their glyph is inspired by the work of Kindlmann [Kin06] with a different parameterization of superellipsoids. Unlike previous work, their parameterization can represent negative uniaxial arrangements and also can represent real symmetric traceless tensors. Positive and negative uniaxial alignments are distinguished by a pinching in the plane orthogonal to the main axes of the glyph. Eigenvalues cannot be used directly for encoding the scale of the glyph due to the traceless nature of the tensor - values may be negative or zero. So other properties of the NLC system are encoded as the axes radii. This paper extends work by Kindlmann [Kin06]

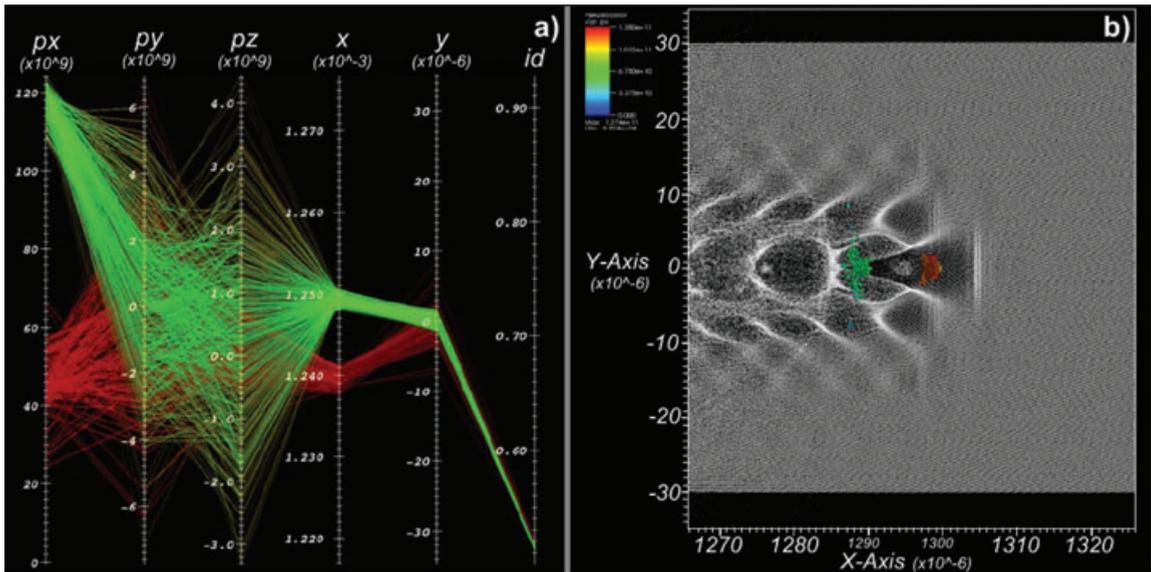


Figure 10: Visualizations for a laser wakefield accelerator simulation. (a) Parallel coordinates and (b) pseudo-colour plot of the beam of accelerated particles. Figure part (a) shows all particles that become accelerated grouped in two separate clusters. The cluster shown in green in part (a) indicates the first beam that is following the laser pulse (the rightmost cluster in part b) and has the highest x -momentum [RPW*08]. Image courtesy of Prabhat.

to represent negative uniaxial arrangements and real symmetric traceless tensors. The method described handles 3D, static data and the main challenge of the paper is multi-field visualization.

Laney *et al.* [LCM*05] present a hardware accelerated, volume rendering based, simulation of radiographs. Their solution can be used as a replacement for software approaches that trades off accuracy for increased performance. They apply their algorithms to the simulation of experimental diagnostics for fusion experiments to optimize simulation parameters. The authors present algorithms for absorption-only and for emissive materials, for hexahedral and tetrahedral meshes. The radiance for a given frequency can be computed by integrating along a linear path through the mesh in a back to front order. The integration is done for a set of frequency bins. The authors extend the GPU volume rendering technique for unstructured grids of Callahan *et al.* [CICS05]. Simulation data is 3D, static on an unstructured grid. The main challenge of the paper is using the GPU to volume render unstructured grids.

As computational power increases, the size of molecular dynamic simulations challenges interactive visualization on workstation computers. Grottel *et al.* [GRDE10] present a method for high-quality visualization of massive molecular dynamics datasets which enables interactive rendering of data containing tens of millions of high-quality glyphs. To obtain interactive rendering the authors employ several optimization strategies. They use data quan-

tization and data caching in the GPU memory (this results in lower CPU-GPU bandwidth consumption). They use coarse, cell-level culling to omit blocks of data from rendering (this results in reduced geometry processing load and lower CPU-GPU bandwidth consumption) and fine, vertex-level culling to omit individual glyphs from rendering (this results in reduced fragment processing load). Rendering is performed using GPU raycasting using deferred shading with smooth normal generation. The authors' work improves on the rendering speed of other molecular dynamics visualization tools such as TexMol [BDST04], BalView [MHLK05], AtomEye [Li03] and VMD [HDS96]. Simulation data is 3D, static and the focus is on efficiently utilizing the GPU for raycasting molecules represented as glyphs.

6.3. Electricity, magnetism and optics

Electricity and magnetism are related physical phenomena associated with electric charges that are stationary (only electricity) or moving (both electricity and magnetism) [bril1a, bril1c].

We outline papers describing techniques that determine the topology of a toroidal magnetic field[SCT*10]* [TGS11].

Optics is the study of the behaviour and properties of light. Geometrical optics deals with tracing of light rays and studies the formation of images by lenses and other optical

devices, and physical optics deals with wave phenomena such as interference and diffraction [bri10g].

We include a paper that visualizes optical power flow through nano-apertures around critical points [SBSH04]*.

Tricoche *et al.* [TGS11] present a general method for the automatic extraction and characterization of topological features in area preserving maps. The authors apply their method to simulation data of the magnetic confinement of plasma in a fusion reactor. Their algorithm extracts fixed points in the map based on island topology, assigns a given range of periods to these features, calculates the Poincaré index for the grid cells that may contain a fixed point, computes the exact information (location, stability type, etc.) of these points, and finally calculates the separatrices that connect the fixed points. The authors extract a topological skeleton of the map and visualize it as a Standard Map (a type of 2D area preserving map). Data mining approaches to identifying features in Poincaré plots through experiment were developed by Bagherjeiran and Kamath [BK06]. Also the new methodology utilizes the work of Andronov [And73] on defining the Poincaré index. The authors present a method for analysing maps with two degrees of freedom of near-integrable systems (i.e. no fully stochastic systems). The main challenge is feature detection for topological features in area preserving maps.

6.4. Gravitation and relativistic mechanics

Historically, the study of gravitation has been placed within mechanics because of Newton's contribution to both areas. The modern theory of gravitation is Einstein's general theory of relativity which accounts for phenomena such as the gravitational bending of light around a massive object [bri10g].

Relativistic mechanics, based on Einstein's special theory of relativity, is concerned with the motion of bodies whose velocities approach the speed of light [bri11d].

We review papers that report on visualizations for theories of general and special relativity [WBE*05]*, [MGW10] and visualize physical aspects of the Gödel universe [GB08]* [GMDW09]*.

See Ruder *et al.* [RWNM08] for an article describing visualization techniques used in physics for visualizing and understanding relativity.

Müller *et al.* [MGW10] present computer simulations of the optical effects of travelling near the speed of light: geometric distortions, Doppler and searchlight effects. Their method provides a different compromise between rendering speed, rendering quality and generality compared with existing relativistic visualization algorithms. There are three methods of rendering objects moving at near light speed: polygon rendering, ray tracing and image-based methods.

Polygon rendering is fast but can introduce visual artefacts that increase with the size of the polygons used to specify a model. Although ray tracing guarantees optimal visual quality it does not work at interactive speeds. Image-based methods are fast but they work only for restricted scenarios where a fast moving observer travels through a static environment. The authors present a hybrid approach based on polygon rendering and local ray casting. They implement their method on the GPU and enable interactive rendering. Their method has fewer artefacts than polygon rendering, is faster than ray tracing and is more flexible than image-based methods by allowing visualization of multiple objects in arbitrary relative motion. They use local ray tracing, see e.g. Reina and Ertl [RE05], to eliminate the object-space search, required in ray tracing to find the triangle intersected by a viewing ray. Müller *et al.* [MGW10] combine work on polygon rendering [HTW90, GMX91] with local GPU ray tracing [Gum03, RE05]. The techniques discussed process 3D, time-dependent, unstructured grid data. The main challenge of the paper is using the GPU for ray tracing.

6.5. Mechanics

Mechanics is the study of the motion of objects under the action of given forces. In classical mechanics laws are formulated for point particles. These laws are extended for bodies with mass distribution in rigid-body dynamics. Elasticity is the mechanics of deformable solids, whereas hydrostatics and hydrodynamics deal with fluids at rest and in motion [bri10g].

This section describes literature that visualizes the turbulent mixing layer between two fluids [LBM*06] and time-dependent foam simulations [LLCD11].

A heavy fluid placed above a light fluid creates a characteristic structure of rising 'bubbles' (light fluid) and falling 'spikes' (heavy fluid) known as the Rayleigh-Taylor instability (RTI). The surfaces separating the mixed fluid from unmixed fluids are known as the envelope and the plane initially separating the two fluids is called the midplane. Laney *et al.* [LBM*06] present a new approach to analyse the RTI by topological analysis of the envelope and of the midplane. The objective is to better understand the physics of the RTI which occurs in many natural and man-made phenomena. The authors extract a segmentation of the upper envelope to identify bubbles using work by Bremer *et al.* [BHEP04] and Bremer and Pascuci [BP07]. They track bubbles over time and highlight merge/split events that form the larger structures at the later stage of mixing of the two fluids using work by Samtaney *et al.* [SSZC94]. They analyse the topology of the density and velocity fields on the midplane to determine if the mixing phases are discernible and to examine asymptotic behaviour at late times. The streaming mesh viewer of Insenburg *et al.* [ILGS03] is used for simplification and viewing of envelope surfaces. Simulation data is 3D, time-dependent, multi-attribute scalar and vector. The main

challenge of the paper is feature detection and tracking where the features are the bubbles of the Rayleigh–Taylor instability.

Lipşa *et al.* [LLCD11] describe the foam research domain area and present an application that provides various techniques for the visualization, exploration, and analysis of time-dependent 2D foam simulation data. The goals are to infer the triggers to various foam behaviours, to visualize general foam behaviour and discover how this behaviour depends on measurable foam properties. The authors parse Surface Evolver[Bra92] simulation data and visualize individual simulation time steps using colour-mapped attribute values enhanced with colour-bar clamping and with a topological changes overlay. Bubbles can be selected and filtered by bubble ID, by location and by attribute value. The time-dependent visualization includes the average for a time window behind the current time step and visualization of bubble paths. Data visualized is 2D, time-dependent on an unstructured grid. The main challenge of the paper is time-dependent visualization, in particular eliminating the large fluctuations in the values of the attributes between time steps determined by changes in the topology of the film network.

7. Discussion and Limitations

Our work has some important limitations to consider. First, because our survey is not comprehensive, it may paint a skewed picture of the current status of research in visualization for the physical sciences. Second, our survey is of a subjective nature as there are a number of valid alternative classifications that can be used to describe the work surveyed. We analyse these limitations next.

We do not review all possible sources that publish visualization work for the physical sciences. Even though we try to be very broad and inclusive, our review is influenced by space limitations and the broad area surveyed. We review papers from the IEEE Vis/InfoVis conferences, EuroVis conference, Supercomputing (SC) conference as well as IEEE TVCG and CGF. We do not review visualization work published in domain specific journals, but rather, we reference surveys, and offer a few examples. All papers reviewed are included in the classification tables, however to address space limitations we only include full summaries for a subset of the reviewed papers. We include a full summary of a paper if the work is recent or if it has a high citation count in Google Scholar.

Whereas visualization solutions may address more than one challenge, we only include in the classification tables the main challenge which highlights the main contribution of the paper.

We do not suggest that our classification is the only way to describe the current state of visualization for the physical sciences. There are a number of good alternative ways to describe it. For instance classifying papers as presentation,

analytical, or exploratory (see Bergeron’s position statement in Visualization Reference Models panel[BAB*93]) is a valid alternative.

Although knowing the current status of research in visualization for the physical sciences is useful, very important drivers in choosing a future research direction include solving a problem, providing a useful tool or addressing a need in the domain science. Domain scientists may provide valuable information on future research directions in their respective fields. Deciding on a future research project in visualization for physical sciences is best done by considering all these factors rather than only the observations offered by our survey.

This paper provides a much-needed starting point. We encourage the reader to use the paper as a way to understand the status of current research and as a first step to explore future work.

8. Directions for Future Work and Conclusions

The status of current work in visualization for the physical sciences presented in Tables 1 and 2 leads us to the following observations. As noted in the Section 7, these observations, when considered alone, might lead to incorrect conclusions. Instead, they should be just one of the many factors that have to be considered when choosing a future research direction.

1. **Multi-field visualization.** Most of the work has been done in earth sciences and physics which suggests that multi-field visualization for astronomy and chemistry may be promising future research directions.
2. **Feature detection.** Locating and tracking features in data is essential for data analysis in many fields of the physical sciences, however most work in this area has been done in physics and chemistry. This suggests that detecting and tracking features for astronomy, and earth sciences may be promising directions of future work.
3. **Graphics hardware.** Most research on efficiently utilizing novel graphics hardware has been focused on chemistry and physics. Using the GPUs in other physical sciences appears a promising research direction.
4. **Scalable visualization** We note that most work has been done for Earth Sciences. Limited computing resources, including resources for visualization, is a perennial problem in the physical sciences. Addressing some of the limitations experienced through scalable visualizations could have the large impact of enabling new analyses and making new discoveries possible.
5. **Error and uncertainty, time-dependent visualization, comparable visualization** A small number of papers address these challenges. They remains top directions for future research in visualization for the physical sciences.

There is also potential for research in the other visualization problem categories proposed by Johnson [Joh04] but not yet addressed in the literature. For example, we believe that integrated problem-solving environments is both relevant and a good research direction for visualization in the physical sciences.

Table 1 reveals that most application papers for the physical sciences visualize 3D static and time-dependent data. The exception is earth sciences where both 2D and 3D time-dependent data is visualized. Most work in astronomy visualizes 3D static data.

There are also opportunities for visualization collaboration in other fields within the physical sciences that have not yet been addressed in the visualization literature, e.g. structural chemistry, geochemistry and quantum mechanics.

In this state-of-the-art report we have provided a comprehensive introduction to visualization solutions for the physical sciences developed in the last nine years. We introduced classifications for the varied visualization solutions provided for physical sciences. These classifications allow us to provide a much-needed global view of this wide area of research. Our survey promotes collaboration with other scientific fields by reviewing recent visualization papers for the physical sciences, by comparing and contrasting them, pointing out how they relate to one another and by classifying them to highlight mature areas, and suggest areas for future work. Through these collaborations, the visualization community can be exposed to new problems and be asked to solve new challenges. In this way, the visualization community can develop innovative techniques to solve our domain experts' problems and keep the visualization field vibrant and relevant for the future.

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