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Visualization for the Physical Sciences

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Abstract

Close collaboration with other scientific fields is seen as an important goal for the visualization community by leading researchers in visualization. Yet, engaging in a scientific collaboration can be challenging. Physical sciences, with its array of research directions, provide many exciting challenges for a visualization scientist which in turn create ample possibilities for collaboration. We present the first survey of its kind that provides a comprehensive view on existing work on visualization for the physical sciences. We introduce a novel classification scheme based on application area, data dimensionality and main challenge addressed and apply this classification scheme to each contribution from the literature. Our classification highlights mature areas in visualization for the physical sciences and suggests directions for future work. Our survey serves as a useful starting point for those interested in visualization for the physical sciences, namely astronomy, chemistry, earth sciences and physics.

Categories and Subject Descriptors (according to ACM CCS): I.3.4 [COMPUTER GRAPHICS]: Graphics Utilities—Application packages

1. Introduction and Motivation

In his influential work, Lorensen \cite{Lor04} reflects on the decrease in the introduction rate 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 to revive the field. Lorensen proposes three main directions through which the field of visualization could obtain a healthy state: (1) Close collaboration with visualization customers can pose challenging problems and expose our community to new and exciting application area, (2) Alliances with other fields, especially computer vision and structural analysis, can generate new synergies, And (3) The definition of some grand challenges can energize our community \cite{Joh04}.

The first proposition inspires us and provides the motivation behind this survey. We review application papers in the physical sciences, classify them in related categories and use the result to identify fields where visualization has been used extensively and fields and areas that may benefit from further exploration.

Ertl \cite{Ert10} argues that the field of visualization is flourishing by citing the overall growth of the number of submissions to main Visualization, Information Visualization and Visual Analytics conferences and by referring to the Visual Analytics initiatives in the US and Europe. In discussing the future of the visualization field, Ertl points out that many visualization techniques are not usable in practice due to complexity of the application and that standard datasets may not be useful for driving our research to relevant applications.

His presentation underscores the view of Lorensen and provides further motivation for our survey. Physical Sciences provide many interesting phenomena which pose new and exciting challenges to visualization researchers. We identify challenges addressed by each paper in our survey. We present the novel techniques used to address those challenges and we classify the papers based on the challenges.

1.1. Visualization for Physical Sciences

According to Encyclopædia Britannica \cite{bri10f}, physical science is the study of the inorganic world while biological science studies the organic world. Physical sciences include astronomy, chemistry, physics and earth 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 the physical scientist may not wish, or be able, to tackle. Off-the-shelf visualization packages, while a great first step in visualizing data, may fail to meet some of the challenges listed earlier. Even more importantly, visualizing data in 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 impact future discoveries and drive innovation in the physical sciences.

We view applications as 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 such that those problems can be solved.

Close collaboration with other scientific fields is seen by leading researchers in visualization [Lor04,Joh04,Ern10] 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. 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 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.

1.2. A Case Study

Complex fluids such as polymer solutions, particulate suspensions or foams provide a good example of a challenging problem. Here is a fluid with microscopic structure that changes in time and changes due to flow. Not withstanding the difficulties in imaging the structure in 3D+time, the rheologist (as researchers in the field of complex fluids call themselves) wishes to understand how the flow of fluids with different material parameters (perhaps different polymer branching, different suspension concentrations, or different bubble sizes) changes. In an unsteady flow, this requires the correlation of elastic and plastic deformation of the structure with local flow-rate/velocity in time.

In the case of foams, we have at least one advantage: the bubbles are sufficiently large (from a few hundred microns to several millimeters in diameter) that they can be imaged fairly directly, and there is a well-defined two-dimensional realization in which the foam is squeezed between two parallel sheets of glass until each bubble spans the gap between them. In this 2D foam it is fairly straightforward to determine the bubble velocities and the visualization of velocity is a choice between vectors and contours, and either a Lagrangian or Eulerian frame. It is also straightforward to see the bubble shapes, but representing spatial and/or temporal averages is a less clear-cut task. One possibility is the texture tensor of Asipauskas et al. [AAG03], where the deformation (as a proxy for the local strain) can be represented by an ellipse with its long axis pointing in the direction of maximum stretch.

All of this presents challenges when, for example, it is required to follow individual bubbles, or small collections of bubbles with certain initial positions or properties, to determine their motion and deformation. Additionally, it is enlightening for the physical scientist to be able to correlate the different measures of material response. Finally, to do this in three dimensions, with the problems of occlusion in the representation and large quantities of data, is a necessary and challenging task.

Figure 1 shows a visualizations of simulated foam flow through a contraction, and the motion of a ball through a 3D foam in a cylinder under gravity. The challenge is to portray the same information as for the visualization of the 2D data for unsteady 3D data: bubble velocity and deformation, local stress, and correlations between them.

2. Classification and Challenges

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 in many different fields and sub-fields, and that some of these fields are overlapping, sometimes papers could be classified in more than one area. For instance, molecular dynamics visualization papers can be classified as chemistry because they visualize organic chemical molecules studied by traditional chemists. However they could be classified as

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biology because those molecules are often studied by biologists.

We have two goals for our classification. We want to to provide a quick but comprehensive picture of the main contribution each paper makes and we want to outline promising directions for future work. A typical classification of visualization techniques [Tel08] (scalar, vector, tensor, . . . ) does not fulfill any of these goals. On the first hand, most of the papers reviewed visualize scalar data which means that we won’t get a good distribution among categories. On the other hand, having many papers using scalar visualization techniques, does not necessarily mean these techniques should not be used to visualize data in the future.

We categorize the literature based on a generic main challenge [Joh04] they address, which also highlights the main contribution of 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 top visualization challenges.

- **Think about the science.** Papers in this category use the science in their respective fields to simulate physical phenomena or to customize visualization techniques to solve a challenging scientific problems. While it is true that most work in visualization uses some domain specific knowledge, visualizations in this category is carried out in close collaboration with the application scientists.

- **Multifield visualization.** Often physical science 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 interaction between those fields is the goal in this category.

- **Efficiently utilizing novel hardware architectures.** The large amounts of data analyzed by scientists can challenge visualization software on several levels: data may be too large to process in real time for visualization, and/or processed data may overwhelm the graphics card capacity to render in real-time. The papers in this category propose novel ways to use the available graphics hardware (GPU) to approach these issues.

- **Feature detection.** Modern sensors and computers produce and store data measured in giga to terabytes. Locating features of interest in these vast amounts of data and tracking the evolution of features in time and/or space are the main goals in this category.

- **Scalable, distributed and grid-based visualization.** This category aims to use scalable algorithms to take advantage of parallel visualization resources available: many graphics cards plugged into the same PC, available on the same cluster or on the grid. The final goal is to produce scalable visualizations that are able to visualize larger data as the amount of resources available is increased.

- **Quantify effectiveness.** The main focus of papers in this category is to compare visualization techniques and to quantify their effectiveness.

- **Represent error and uncertainty.** Measurement or simulation errors are part of the data analyzed by physical scientists. The main focus for papers in this category is integration of error visualization in the main visualization of data.

- **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.

Table 1 presents an overview and classification of visualization work in the physical sciences. Papers are grouped by domain along the x-axis and by the main challenge or contribution along the y-axis. Each entry is colored according to the temporal and spatial dimensionality of the data. Entries are also ordered chronologically within each sub-group. This table provides an at-a-glance global picture of research in visualization for the physical sciences. It highlights both problems for which a number of solutions have been provided and directions for future research.

Table 2 presents an alternate classification for visualization work for the physical sciences. Papers are grouped by domain along the x-axis and the temporal and spatial dimensionality of the data along the y-axis. Entries are also ordered chronologically within each sub-group. This table highlights the dimensionality of the data where most work has been done.
### Table 1: An overview and classification of visualization research in the physical sciences.

Papers are organized by domain along the x-axis and by the main challenge addressed along y-axis. 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 color scheme is blue for 2D, static data, green for 2D, time-dependent data, yellow for 3D, static data and red for 3D, time-dependent data. Finally, entries are ordered in chronological order within each group. This table provides an quick overview of research, it highlights challenges for which a number of solutions have been provided as well as directions for future research.

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2.1. Overview

Papers in the think about the science category make use of domain specific knowledge to visualize data or simulate physical phenomena. The science of sound is used in simulating sound reflection and refraction within the room [BDM*05, LCM07b, CLT*08, BMD*08, DBM*06] and these simulations are used to study the influence of the room geometry and walls’ material on the sound perception by a listener [BDM*06, MDHB*07] inside the room. Edelsbrunner [Ede99] defines a macromolecule skin surface model which is better than the existing models [CS04]. This paper generates further interesting work to triangulate that surface [CS04, CS05]. Jimenez et al. [JCSB03] adds advanced interactive 3D visualization tools to a complex environmental observation and forecasting system for the Columbia River, Sun et al. [SBSH04] visualizes the optical power flow through a C-Shaped nano-aperture, Song et al. [SYS*06] visualize warm rain formation and Navratil et al. [NJB07] visualize the formation of the first stars.

These papers take advantage of advanced domain knowledge and/or close collaboration with the physical scientists to advance the domain specific and the visualization field. Weiskopf et al. create explanatory and illustrative visualizations to communicate theories of general and special relativity [WBE*05] while Grave et al. [GB08, GMDW09] visualize physical aspects of the Gödel universe.

For multifield visualization in the physical sciences, a number of solutions have been provided. Realistic visualization of physical phenomena use multifield data from simulation or acquired through non-visual means and aim to visualize this data in a visually realistic way. These visualizations may appeal to scientists used to gather data through visual inspection [REHL03], may be used for comparison with data acquired with video cameras [SBS*04] or for producing scientifically accurate animations for educational purposes [MHLH05]. We believe realistic rendering of phenomena may be useful to a wide range of physical scientists so we think this is a good direction for future research.

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Table 2: An alternate classification of visualization research in the physical sciences. Papers are organized by domain along the x-axis and by the dimensionality of the data along the y-axis. Entries are ordered in chronological order within each group. This table provides an quick overview of research, it highlights the dimensionality of the data where most work has been done, as well as possible directions for future research.

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Multi-field, 2D data is visualized using a field as a third dimension and using either volume rendering or stacked visualizations of each field [LHF08]. Multi-field 3D data is visualized using glyphs and a variation in the glyph color [SIG05] or shape [CFG05, BvL06, JKM06], parallel coordinates [QCX07] or multiple-linked views and brushing [CFG05, KLM08]. 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 source characteristics [SB04]. While this is an appealing challenge, many challenges remain such as meaningful mapping between field values and sounds, generating pleasant sounds and the speed of processing.

Most papers that use novel hardware architectures (GPUs) are from chemistry (or physics) and visualize molecules [BDST04, RE05, TCM06, GRDE10], molecular surfaces [KBE09, LBPH10] or quantum chemistry simulations [QEE05, JVM09]. From astronomy, work by Fraedrich et al. [FSW09] visualizes large particle-based cosmological simulations. We believe other physical sciences could benefit from using novel hardware architectures for improved computation and rendering speed.

Papers that have feature detection as their main goal are varied. Locating important features within the data uses domain specific knowledge. We review techniques that recover the structure of planetary nebulae from 2D images [MKDH04], examine structures defined by intercluster galaxies [MQF06], detect anomalous structures in molecular dynamics simulation data [MHM04] or in nematic liquid crystals [MJK06, SPL06], calculate the lines that separate rocks with different mineral densities or porosity characteristics [PGT08] and identify regions in the atmosphere which can act as indicators for climate change [JBMS09]. Two papers approach both feature detection and feature tracking. Bidmon et al. [BBG08] track and visualize the paths of solvent molecules [BBG08] and Laney et al. [LBM06] identify and track the surfaces separating a heavy fluid placed on top of a light fluid.

Few scalable, distributed and grid-based visualization have been proposed for the physical sciences. Qiao et al. [QMK06] present a novel remote visualization framework for the nanoHUB.org while Stainforth et al. describe visualization for public-resource climate modeling [SFW04]. We believe this is a promising area of future research.

There is one paper that focuses on quantifying the effectiveness of visualization techniques. Bigler et al. [BGG06] explain and evaluate two methods of augmenting the visualization of particle data. However, their evaluation is informal, using feedback from the application scientists.

Li et al. [LFLH07] present tools and techniques for visualizing error and uncertainty in large scale astrophysical environments. We believe representing error/uncertainty in other visualizations for physical sciences is an important area of future research.

There is one paper that focuses on global/local visualization (details within context). Li et al. [LFH06] present a set of techniques to facilitate travel and context acquisition in an astronomical virtual environment. A few papers [KLM08, CFG05, LFH08] from the Multifield visualization category include interactive brushing, which shows details within the context. While the visualization community would benefit from research for visualizing details within context [Joh04] it is unclear what contribution visualization for physical sciences would have to this research.

Most of the papers reviewed visualize either 3D static or 3D dynamic data. We review only one paper in astronomy that visualizes 2D static data [LFH08] and two papers in climatology [JBMS09] and in atmospheric sciences that visualize 2D time-dependent data. We believe the reasons behind this fact are that scientists have the tools and the know how to visualize data in 2D but not in 3D and that visualizing data in 2D is inherently easier.

Figure 2 shows the overall frequency of visualization papers in the physical sciences published at the Vis and EuroVis conferences in the last eight years. We note the very recent decrease in the number of visualization papers in the physical sciences. While the reasons behind this decrease are beyond the scope of this paper we believe there are plenty of promising opportunities to create quality work in visualization for the physical sciences.

2.2. Contributions and Summary

The main benefits and contributions of this paper are: 1. We review the latest developments in visualization for the physical sciences; 2. This is the first survey of its kind that provides a comprehensive view on existing work on visualization for the physical sciences; 3. We introduce a novel classification scheme based on application area, challenges...
addressed and data dimensionality and apply this classification scheme to each contribution; 4. Our classification highlights mature areas in visualization for the physical sciences where many solutions have been provided and suggests areas where visualization could have a contribution at advancing the science. These areas can potentially introduce new exciting problems to the visualization field and can contribute to its advancement.

This is not simply a list of papers. The relationship between papers is also explored and described. The contributions of each is presented in the context of closely related work. The rest of the paper is organized as follows: we review visualization papers for astronomy (Section 3), for chemistry (Section 4), for earth sciences (Section 5), for physics (Section 6) and we end with directions for future work and conclusions (Section 7).

3. Astronomy

Astronomy is the science of the entire universe which includes the study of planets, stars, galaxies, nebulae and interstellar medium. Astronomy and physics are linked through cosmological theories based on the theory of relativity [br10a].

This section presents papers that describe visualizations of nebulae [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 [LFDH06], visualize uncertainty in astrophysical data [LFDH07], visualize the formation of the first stars [NIB07], multifield sky data [LFDH08] and cosmological simulations studying matter distribution in the universe [FSW09].

Auralization is the process of extracting meaningful information from data and displaying it in form of sound. Shin et al. [SB04] introduce a field auralization technique whose objective is sound synthesis from a 3D time-varying volumetric data. This sound data is used for augmenting visualization for enhanced perception and understanding of cosmological explosions. First density and density gradient in the field data is mapped onto acoustic parameters density and particle velocity. Vertices are categorized as monopole, dipole or quadrupole sound sources based on the pressure and velocity values at those vertices. Finally, pressure as a function of time and of listener position is calculated for all three types of sound sources. Both parameter mapping and direct simulation auralization examples are offered in work by McCabe [MR94]. This work takes a hybrid approach between parameter mapping and direct simulation by mapping parameters of the data to acoustic parameters and then using simulation to find the sound at the listener position. This work processes 3D, time-dependent data and the main challenge is using the science of sound.

Figure 3: Planning a travel path from Centauri Proxima ($10^{-7}$) to Earth ($10^{11}$) using logarithmically mapped eye space [LFDH06].

Miller et al. [MQF06] present an interactive visualization tool used to examine structures defined by intercluster galaxies within the Horologium-Reticulum supercluster (HRS), one of the largest conglomerations of visible and dark matter in the local universe. Galaxies and galaxy clusters within HRS are represented as point data. Glyphs are used to represent galaxies and galaxy clusters. Users can partition galaxies and color code them based on group membership. Right Ascension-Declination-recessional velocity (RA-DEC-cz) reference axis are displayed for orientation within the data and projection lines can be displayed for galaxies to relate 3D data with the 2D projections astronomers are used to. Torsional rocking, which mimics the motion of a torsional pendulum and stereo view are provided to complement the depth perception provided by camera motion. AstroMD [GBCB02] is a astronomical and visualization tool closely related to this work that has numerous visualization techniques but it does not provide interactive partitioning of galaxies and projection lines. Data processed is 3D, static, and the main focus of the paper is feature detection.

The visible universe spans a huge range of distances and it 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. [LFDH06] present a set of techniques to facilitate travel and context acquisition in an astronomic virtual environment (see Figure 3). Navigation and object representation in the multi-scale universe is done using power spatial scaling described in the authors’ previous work [FH07]. This technique scales the entire Universe’s data relative to the current view scale. The authors use a 3D compass for orientation reference and annotated 3D land-
marks for context. They use a cube, cylinder or sphere as power cues to show the current image scale and they use as a proximity cue an edge which fades in when an object is close to the viewpoint. Li et al. [LFH06] use as an overview map 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. 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. The authors present tools for visualizing uncertainty in astrophysics. These tools include: a unified color 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, 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 in Li et al. [LPH06] and Fu et al. [FH07] by adding uncertainty visualization to the presented astrophysical visualization tools. The algorithm presented processes 3D, static data and the main challenge is representing error and uncertainty.

Navrátil et al. [NJB07] describe a visualization process for a particle based simulation of the formation of the first stars. Their visualizations provide insight into the evolution of the early universe and guide future telescope observations. The authors use numerical simulation [SH02, SYW01], which involve three-dimensional 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 can be characterized as $n^{th}$ nearest neighbor density estimate and as localized inverted weighted distance interpolation. It 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. Navrátil et al. use an interpolation algorithm from computer graphics [Jen96, JC98] and ParaView’s isosurface extraction and smoothing functionality to generate novel visualizations of the first stars formation. Simulation data is 3D, time-dependent. The main challenge of the paper is learning the meaning of the simulation data.

Li et al. [LFH08] propose visualization and exploration of astrophysical data using a third dimension corresponding to a broad electromagnetic spectrum coming from a wide range of all-sky surveys. Light of different wavelengths is obtained from a variety of detector sources. A preprocessing step is applied to obtain uniform representation and units of measure before visualization and exploration of data. Data is visualized using textured image stacks (presented linearly or using the horseshoe representation) or volume visualization (GPU-based). Data is explored by using interactive data mapping, mini-map explorer and interactive feature analysis (brushing) (see Figure 4). Brugel et al. [BDA93] examined multi-spectral data with a limited spectral range and Jacob et al. [JP01] focused on information extraction from multi-spectral astrophysical data. Li et al. [LFH08] propose a general visualization framework which processes a broader spectral range. Sky data is 2D, static while the main focus of the paper is multifield visualization.

Fraedrich et al. [FSW09] explore scalability limitations in the visualization of large particle-based cosmological simulations and present techniques to reduce these 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. For reducing disk access latency impact the authors use asynchronous I/O and prefetching. The authors use a vertex array buffer to store data on the GPU and a vertex shader to render the data (see Figure 5). Particle data from cosmological simulation is rendered in software by Dolag et al. [DRGH08]. 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 a first approach that is able to interactively visualize particle data exceeding 10 billion elements. Simulation data is 3D, static and the main challenge is efficiently using novel hardware architectures.

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4. Chemistry

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

4.1. Nanotechnology

Nanotechnology is the manipulation of atoms, molecules and materials to form structures at nanometer scales. These structures typically have new properties than 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 present a web based nanotechnology visualization tool [QMK’06].

Saunders et al. [SIG05] present several point-based techniques for the visualization of the formation of nanoparticles in turbulent flows. The points are used with different rendered attributes such to visualize several values in the same image. The mean diameter and standard deviation of the particles are visualized together. The paper presents a series of implementations of different techniques. The principle technique is that a glyph is used to represent the data. Multiple values are represented through perceptually equiluminant color-scales. One of the challenges addressed is to work out how to place the glyphs such that no perceptual bias is given to either large values or smaller points. This is achieved through (i) generating a regular grid of potential point locations and (ii) jittering prospective spot locations. (iii) For each potential spot location the footprint of candidate spot is calculated; (iv) Any spot that overlaps existing spots is thrown away. (v) move to next spot location. The main areas of related work is artistic rendering of scientific data by glyphs, such as Laidlaw et al. [LAK’98] and Kirby et. al [KML99]. Dimensionality is 3D, time-dependent, uniform resolution, regular grid, scalar data. The main focus of the paper is multifield visualization.

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 grid supercomputing resources and use remote hardware accelerated graphics for visualization from a within a web browser. The authors created nanoVIS a visualization engine library that can handle a variety of nanoscience visualizations involving vector flows and multivariate 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. nanoVIS visualization engine uses work by Qiao et al. [QEE’05] for visualization of multivariate scalar fields using texture-based volume rendering and work by Kolb et al. [KLR04] and Kruger et al. [KKK’05] 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, distributed and grid-based 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 visualizations of quantum chemistry simulations [QEE’05, JVM’09].

Qiao et al. [QEE’05] describe a method and system for visualizing data from quantum dot simulations. The output from these simulations is in the form of two Face-Centered Cubic lattices (FCC), which are not handled well by existing systems. A hardware-accelerated volume rendering approach and application are described and demonstrated. Decomposing the FCC lattice can result in an enormous number of tetrahedra, which makes rendering multi-million atom
simulations difficult. By using a 3D texturing approach with a logarithmic transfer function, interactivity is achieved. The software can also render multiple fields at once, and perform GPGPU statistical calculations on the selected data. Builds on the approach of Rober et al. [RHE03] for BCC (body-centered cubic) grids and Westerman and Ertl’s work on 3D texturing [WE98], and computes statistics 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 focus is on efficiently using the GPU.

Jang et al. [JVM+09] visualize results from quantum chemistry computations without resampling the data in a grid structure. This technique results in improved rendering speed and less GPU memory needed than current visualization tools for quantum chemistry. The volume visualization tool described handles direct evaluation of functions using a GPU fragment program. Only functions’ parameters are stored and transferred to the GPU. This saves transfer time to the GPU and GPU memory compared with current tools which store data in a grid. Jang et al. [JWH+04, JBL+06] present a technique to procedurally encode 3D scalar data and reconstruct this data on the GPU. This technique eliminates the need for a large grid or mesh to be used for rendering. The authors extent that work for visualizations for quantum chemistry. Quantum chemistry data is 3D, static, scalar and the main focus is on efficiently utilizing the GPU.

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 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 [LBPH10, KBE09], generate triangulations of molecular surfaces [CS04, CS05], visualize solvent pathlines near protein cavities [BGB+08], detect anomalous structures in molecular dynamics simulation data [MMH+04].

Bajaj et al. [BDST04] describe both an application that uses programmable graphics units 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. 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 allow 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 novel hardware architectures.

Mehta et al. [MMH+04] seek to detect anomalous (non-ideal) structures in principally 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) convolve with a band-pass filter to amplify the high frequency component. (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 neighbor analysis (CNA) [CJ93] or solely visualization [VBM+95]. This article 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.

Cheng et al. [CS04] present a new skin model of molecules, an implicit surface, using an advancing front surface method that constructs a Restricted Delaunay Triangulation over the model surfaces. The surfaces are calculated directly from a van der Waals force model. The challenge is to create skin mesh models that are of good quality, provable to be correct, fast to compute and the algorithm completes. Their approach is to use an advancing front surface method. 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 the curvature of the surface as the surface advances. 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 geometry. Data processed is 3D, static, uniform resolution - but the size of triangles is determined by the curvature, no explicit grid, 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 meshes for molecular surface models. This is the first robust algorithm that is capable of generat-
ing molecular surface meshes with guaranteed quality. The authors generate a mesh for the skin surface incrementally. They add one sample point then update the Delaunay triangulation. They extract a candidate surface. If more points can be added, the algorithm proceeds to the next step, otherwise the algorithm finishes. The algorithm produces a Delaunay triangulation of a ε-sampling of the molecular surface with guaranteed quality (minimum angle of any triangle) This paper extends work by Cheng et al. [CDES01] by improving the efficiency of the algorithm. The algorithms presented handle 3D, static data and the main challenge is generating a mesh for a molecular surface model.

Tarin et al. [TCM06] present a set of techniques to enhance the real-time visualization of molecules. These techniques enhance the user’s understanding of the 3D structure 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 meaning that all attributes are synthesized on the fly. A vertex program expands the impostor producing all fragments for the front face of the primitive, a fragment program computes texture position, depth or lighting. 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 effect 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] and by Pharr [PG04]. The techniques described handle 3D, static, unstructured grid data and the main challenge is how to efficiently use the GPU.

Bidmon et al. [BGB*08] present a novel visualization of molecular dynamics simulations that shows the solvent paths (water) entering and exiting the cavities of a protein. They track the solvent molecules only inside a region of interest (ROI), which is a sphere around the protein. They filter out solvent molecules that pass the ROI with high velocity, and solvent molecules outside of the protein. They filter out the small-scale, chaotic movement of the molecules by applying a smoothing operator to the pathline. When rendering the pathlines, additional information is conveyed by mapping the position in time of solvent molecules to a color and the velocity to the saturation of the color. To reduce the number of paths, adjacent pathlines with similar dynamic properties are merged together. Pathlines are represented using cubic Bézier curves. Clustering the pathlines and visualization can be changed dynamically by the viewer. The authors extend the work by Bakowies and Van Gunsteren [BVG02] by visualizing pathways inside the cavity and providing information if water molecule enter and exit the cavity by the same exit. Pathlines are clustered and visualized as tubes as in work by Telea and Van Wijk [TVW99]. Tracking solvent atoms over their trajectories is done by Visual Molecular Dynamics software [HDS96]. Bakowies and Van Gunsteren [BVG02] identify protein cavities and statistics are calculated that describe which exit the water molecule takes out of these cavities. The results are demonstrated on 3D, time-dependent, unstructured grid, vector attributes. The main focus of the paper is feature detection.

Krone et al. [KBE09] present a new 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 (see Figure 6). For rendering the SES the authors use Sanners’s Reduced Surface [SOS98] because it requires straightforward computation and simplifies processing for dynamic data. Krone et al. use acceleration techniques to achieve interactive frame rates for rendering long trajectories. These techniques are filtering out unwanted protein motion which was introduced by Kabsch et al. [Kab76] and semantic reduction of the raw atomic data as in work by Bond et al. [BHI*07]. The authors use several common visualization techniques for enhanced protein analysis. Connolly [Con83] presented the equations to compute SES analytically. Sanner [SOS98] developed the Reduced Surface which accelerates the computation of SES. Chavent et al. [CLM08] present a related visualization application 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 while the main challenge addressed is how to efficiently utilize the GPU.

Lindow et al. [LBPH10] present ways to accelerate the construction and the rendering of solvent excluded surfaces (SES) and molecular skin surface (MSS) which are used
in visualizing the dynamic behavior of molecules and gaining insights into a molecular system. 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 using 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 and the challenge is efficiently utilizing the GPU.

5. Earth Sciences

Earth sciences study the solid earth (geologic sciences), its waters (hydrologic sciences), the air around it (atmospheric sciences) and their evolution in time [br10d]. It consists of many disciplines which include the study of water on and within the ground, glaciers and the ice caps, the oceans, the atmosphere and its phenomena, the world’s climate, physical and chemical makeup of the solid earth, study of landform and the geologic history of the Earth.

5.1. Atmospheric sciences

Atmospheric sciences deal with properties, structure and composition of the atmosphere, understanding atmospheric phenomena such as clouds, fog and dew, understanding weather changes and the ability to do accurate weather forecasting.

We present papers that visualize cloud scale weather data [REHL03], visualize warm rain formation and compare weather models with radar observation [SYS*06] and analyze air pollution [QCX*07].

Riley et al. [REHL03] describe a system for visually accurate presentation of storm and cloud scale multi-field weather data. Meteorologists are trained to extract information about a forming storm through visual observation. The goal of this work is to maximize comprehension of data though presentation in a visually accurate fashion. A storm cloud is comprised of many water particles of various states, sizes and shapes. Particles considered by this work are: cloud, ice, rain, snow and soft hail. Simulation data provides the concentration of each kind of particle in a cloud. This data is volume rendered [NDN96] on the GPU using a translucency model described by Kniss et al [KPH*03]. This work extends cloud rendering techniques [NDN96] to storm and cloud scale weather visualization. It uses the translucent model described by Kniss et al. [KPH*03] for multiple scattering. The system described handles 3D, time-dependent data and the challenge is multifield visualization.

Song et al. [SYS*06] present an atmospheric visual analysis and exploration system for weather data. The system enables integrated visualization of atmospheric data sets from different sources using a variety of rendering techniques. The application is used for gaining insight into warm rain formation in small cumulus clouds and for validating severe storm models by correlate visualization of a storm model and of experimental Doppler storm data. The system described by the authors can fuse datasets from a wide range of sources, scales and grid structures [RSK*06]. It uses physics-based rendering of clouds [REHL03], illustrative rendering of the attribute data using either 1D or 2D transfer functions, allows for visualizing synthesized attributes which are functions of existing attributes and it has an editable transfer function interface. Work by Riley et al. [RSK*06] is used to fuse data sets from a wide range of scales and grid structures. Work by Riley et al. [REHL03] is used to provide physically-based, visually accurate cloud rendering. Weather phenomena are 3D, time-dependent, multi-attribute, both scalar and vector and multiple grid types. The main challenge of the paper is learning the specifics of weather data and working closely with the domain scientists.

Qu et al. [QCX*07] present a weather data visualization system used for analyzing the Hong Kong air pollution problem. The system visualizes attributes describing air quality and allows the exploration of correlations between these attributes. Wind speed and direction are main attributes that drive the exploration of other attributes which 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. The value of the attribute is shown using a color map. A sector of interest can be selected from the polar coordinate display. Using this sector a pixel bar chart [KHD02] is shown which depicts three additional attributes (axes X, Y and color) for a certain wind direction and speed. Data can be explored using parallel coordinates [ID90]. Correlation between attributes is computed using the correlation coefficient [QCX*07] which can detect linear dependencies for normally distributed data. A weighted complete graph is used to show this correlation. Work by Barnes and Hut [BH86] and Noack [Noa05] is used to draw the graph such that the distance between nodes reflects the strengths 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, color mapping, parallel coordinates and pixel bar charts to visualizing air

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quality measures in Hong Kong and exploring their correlation. The phenomena being studied is 2D, time-dependent, scalar, multi-attribute on an unstructured grid. The main challenge of the paper is multifield visualization.

5.2. Climatology

Climatology [bri10c] is concerned with climate differences between different regions and climate changes in long periods of time. Climatology seeks to identify slow acting influences on climate and tries to identify practical consequences of climate change.

We review papers that visualize climate variability changes [JBMS09], identify regions in the atmosphere which act as indicators for climate change [KLM’08] and describe visualization for public-resource climate modeling [SFW04].

Kehrer et al. [KLM’08] demonstrate the use of visualization and interaction technologies for identifying regions in the atmosphere which 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 synthesised 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 SimVis [DGH03, DH02, DMG’04, MKO’08] framework for climate research. Extensions to the 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.

Jänicke et al. [JBMS09] explore ways to assist the user in the analysis of variability of a global climate model data. Changes in frequency or the spatial patterns of natural climate variations are highlighted as possible evidence of climate change (see Figure 7). The authors use three techniques to provide a more abstract representation of the wavelet decomposition information [TC98]. Scalar characteristics are extracted and displayed using a color map, regions with similar patterns are clustered enabling information-assisted interaction and reoccurring patterns in different places of the dataset are identified using similarity fields. Works by Lau and Weng [LW95], Sonechkin and Datsenko [SD00] and Pišoft et al. [PKB04] use wavelet analysis to investigate climate change, but only for a small number of time series. The authors explore different techniques to make wavelet applicable to an entire multivariate climate dataset with a grid size 200 × 100 and 3000 steps that would otherwise result in 20000 graphs to be analyzed. The techniques described handle 2D, time-dependent, multi-attribute scalar data on a structured grid. The main challenge of the paper is feature detection.

5.3. Hydrology

Hydrology studies the waters of the Earth, their distribution and circulation as well as their chemical and physical properties.

We describe a study that describes visualization tools for an environmental observation and forecasting system for the Columbia River [JCSB03].

The paper aims to bridge the gap between the predominantly two-dimensional oceanographic visualization tools and the three-dimensional visualization tools that are not specific to the needs of the oceanographer. The resolution of the current three dimensional visualizations that are currently used are low compared with the high quality and multi-resolution models that are generated by the simulation capabilities of the CORIE system. 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 the close collaboration with the physical scientists.

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
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 sciences 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 not only the phenomena responsible for the sensation of hearing but also includes sounds with frequency too high or too low for the human ear and also transmission of sound through other media than air [Pie89].

We review papers that physically simulate sound within a room [BDM’05], [LCM07b, CLT’08, BMD’08], show how material on a room surfaces influences sound coming from a source [DMB’06, MDHB’07], 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 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). A BRDF is then 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], computationally expensive and receiver-location dependent. Processed data is 3D, time-dependent. The main challenge of the paper is performing the sound simulation.

Deines et al. [DBM’06] present visualizations of acoustic behavior inside a room. Through these visualizations the authors’ show the surface material 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. These techniques are based on phonon tracing [BDM’05], the authors’ previous work on acoustic simulation. The authors present four visualizations techniques for acoustic behavior. They visualize phonons on surfaces by rendering each phonon as a sphere and color coding it according to its spectral energy. A second technique visualizes wave fronts reflected at the room surfaces by clustering phonons with common history and color coding the resulting surface based on the energy of the phonons. The phonon clusters reduce to just a phonon as the number of reflections increases so this technique works only for visualizing wave fronts of phonons resulted from a few reflections. A third technique produces a

\[\text{Figure 8: Blending from illustrative rendering to uninterpreted data rendering for seismic volumetric reflection data. [PGTG07].}\]
continuous representation of the emitted energy on the surfaces of the room by interpolating on the energy and path-length of the phonons. Finally, a forth technique shows a deformed sphere according to the amount of energy received from various directions color coded based on the frequency of the sound received. Deines et al. [DBM’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 a unstructured grid. The main challenge is using the science of sound to perform and use the simulation.

Deines et al. [DBM’06] present a comparative visualization of two different approaches for acoustic simulation. The first approach is a finite element based solution (FEM) of the sound wave equation which is very precise but is computationally intensive at medium and high frequencies. The second method, called phonon tracing, is more efficient than FEM at medium and high frequencies but is 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. These results can be used for combining the two acoustic simulation methods by using the FEM method at low frequencies and using phonon tracing at medium and high frequencies. The authors present an improved version of their previous method, phonon tracing [BDM’05], as one of acoustic simulations approaches. The improvement consists of using pressure instead of energy for calculations which facilitates comparison with FEM algorithm. Phonon tracing works by tracing sound particles from the source sound through a scene and building a phonon map on the scene geometry. After that, the phonons are collected at the listener position in order to calculate the room impulse response. Phonon tracing fails in the low frequency range due to diffraction and interference effects, so wave acoustics is used to simulate the low frequency part of the sound field. The wave equation is solved by finite element method (FEM) which 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 and they visualize the interference patterns and wave propagation for different frequencies of the signal. The also visualize the gain and for both simulation methods and difference between them. 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. They use phonon tracing together with a FEM simulation and they visually compare the two methods at different frequency ranges. The phenomena begin studied is 3D, time dependent, on a unstructured grid. The main challenge is using the science of sound for acoustic simulation.

Michel et al. [MDHB’07] visualize the importance of scene surfaces for the sound quality at different listener positions or the complete audience. Importance denotes how much a certain scene surface contributes to the sound quality measure. This visualization gives clear advice on which parts of the room geometry need to be changed (by changing the material) to improve the chosen acoustic metric. The authors use their system for the improvement of speech comprehensibility in a lecture hall at university (see Figure 9). Michel et al. [MDHB’07] use the phonon tracing algorithm [BDM’05, DBM’06] to produce sound simulation data. The phonon tracing algorithm consists of two steps: phonon emission which calculates particle traces and stores phonons on all reflecting surfaces and phonon collection which calculates the contribution of each phonon (point on the room geometry) to the total pressure and energy at the listener position. The comprehensibility of human speech is assessed by computing the ratio between early reflections which is sound arrived at listener position within a certain time range (50 ms) and late reflections which is sound arrived at listener position after a certain time passes (50 ms). The authors present two visualizations: They use glyphs to show and compare early and late reflections at listeners positions as in work by [SG89]. The use color mapping to show the contribution of each point in the geometry to early and late reflections for individual listener positions or for the whole audience. The authors extend work by Bertram et al. [BDM’05] and its subsequent improvement by Deines et al. [DBM’06] with visualizations used to assess sound quality in a room and to give advice on which parts of the room need to be changed to improve the measured sound metric. Sound data is 3D, time-dependent, multi-attribute on a unstructured grid. The main challenge is using the science of sound for acoustic simulation.

Lauterbach et al. [LCM07b] present a new algorithm for interactive sound rendering which can handle complex scenes with tens or hundreds of thousands of triangles, dynamic sound sources and dynamic objects. The authors follow sound 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
Figure 10: Phase visualization of sound received at one listener position for the first reflection. [BMD*08]. Image courtesy of

scene triangle is calculated. Beam tracing calculates the exact intersection. In frustum tracing, the frustum is subdivided uniformly in smaller sub-frusta and only discrete clipping is performed at the sub-frusta level. The algorithm described by Lauterbach et al. [LCM07b] can be thought 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. As before, the main challenge is doing the acoustic simulation.

Bellman et al. [BMD*08] present a visualization of acoustic pressure fields on a scene with acoustic reflection and scattering. Their method facilitates the evaluation of simulated acoustics which is complementary to auditive evaluation (see Figure 10). Bellman et al. [BMD*08] present a pressure-based acoustic rendering equation and a corresponding ray-tracing method for simulating a room acoustics. The authors use recursive ray-tracing to calculate sound pressure (amplitude and phase) at any point in the room. Bertram et al. [BDM*05] visualize the sound wave propagation by the use of color coded spheres representing phonons. Deines et al. [DBM*06] introduce the phonon tracing method and in previous work [DBM*06] they visualize wave fronts on the scene surfaces using the phonon map. Michel et al. [MDH*07] analyze the acoustic quality at a listener position. Previous visualizations are based on graphical primitives and do not make use of an acoustic rendering equation. Data processed is a sound function at the source and a multi-attribute description of the room. The algorithms presented process 3D, time-dependent, multi-attribute data on an unstructured grid. The main challenge of the paper is doing 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 modeling, multi-sensory visualization and training system. Their algorithm can offer considerable speed-ups 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 modeling. Sound data is 3D, time-dependent, multi-attribute scalar, unstructured grid and the main challenge of the paper is using the science of sound to do the sound simulation.

6.2. Atomic and Chemical Physics

Atomic and Chemical Physics studies matter on the smallest scale at which chemical elements can be identified. Most important properties of matter that are encountered in normal experience depend only on the mass of the atomic nucleus and its charge [br10g,col07].

We present research that visualize particle data generated by accelerator modeling simulations [CFG*05], defects in nematic liquid crystals [SPL*06, MKJ06] and nematic liquid crystal alignment [JKM06] and visualize large molecular dynamics simulations [RE05, GRDE10]. We review a paper that visualize Fourier transform mass spectrometry experiments [BvL06].

Particle physicists rely heavily on simulation and data analysis to aid design before committing to construction of expensive particle accelerators. They need effective visualization capabilities to aid this process. Co et al. [CFG*05] enable physicists to gain a better understanding of their data by creating tools that allows them to interact with multiple plots of the data. 2D and 3D scatterplots are linked for selection, and disc orientation is used to show additional attributes in a manner similar with surflets [PZVBG00]. While little is new in the features offered, the system as a whole is described as effective. The painting interface is similar to [TM03, DGH03], the orientation of discs in 3D views is essentially the method of Pfister et al. [PZVBG00]. The best-known tool in the field, [CER02], is described as lacking the ability to select and track points over time. Simulation data is 3D, time-dependent, uniform resolution. The main challenge addressed by the paper is multifield visualization.

Reina et al. [RE05] describe a method for visualizing thermodynamic simulations using the GPU that minimizes the quantity of data that needs to be transferred by generating

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implicit surfaces directly in the fragment program. This approach improves both visual quality and performance (in frame-rate terms). 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 utilizing the GPU.

Grottel et al. [GRDE10] present a method for high-quality visualization of massive dynamic datasets which allows for 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 quantization and data caching in video memory. They use a coarse culling via hardware occlusion queries and vertex-level culling using maximum depth mipmap. Rendering is performed using GPU raycasting using deferred shading with smooth normal generation. The biggest shared of performance increase is due to the data transfer reduction between the main memory and the GPU due to coarse occlusion culling on the grid cell level. The authors work improves on the rendering speed of other molecular dynamics visualization tools such as TexMol [BDST04], BallView [MHLK05], AtomEye [Li03] and VMD [HDS96]. Simulation data is 3D, static and the focus is on efficiently utilizing the GPU.

Slavin et al. [SPL*06] aim to visualize defects in liquid crystals. In particular the nematic (thread-like) state of the crystals. They use several visualization methods to address specific research questions. The simulated discrete molecular data is sampled (using a cubic B-spline kernel) onto a regular grid, where each point is a tensor. Using AVS, streamtubes are shown over integral paths that are calculated through the principal eigenvector field. Possible locations for defects occur when the molecule ordering is low (there are no streamtubes) and values of small linear anisotropy (shown by isosurfaces). Colors were also added to the tensor values of the tubes, and users could probe specific points to understand qualitative values. The focus of the visualization is to use streamtubes and surfaces [SPL*04]. The techniques described work on 3D, static, uniform resolution, tensor data. The main focus of the paper is feature detection.

Burakiewicz and van Liere [BvL06] present visualizations of simulations of Fourier transform mass spectrometry (FTMS) experiments. Instead of rendering particle position data directly onto the screen as points or glyphs, the authors first extract motion information from the ion position data and then map this information onto geometric primitives. This reflects how physicists think about their data and avoids the cluttered images the would result from direct visualization. Visualization based analysis of FTMS simulations is used to further improve the resolution and mass accuracy of Fourier transform mass spectrometry devices that play a leading role in biological mass spectrometry. The authors use three visualization idioms to capture essential properties of the data. First they cluster ions whose mass to charge ratio belongs to a user defined interval. A cluster is rendered as a comet icon with thickness encoding the density of the ions in the cluster, and the length of the comet showing dephasing of the ions in the cluster. Second, they use a frequency icon to show the difference between measured group’s cyclotron frequency and expected cyclotron frequency and they use a dephase icon to encode dephasing information of a cluster. Third, they use camera control for analyzing relative motion of an ion cluster, by positioning the camera relative to that cluster. Most particle visualizations directly render particle data as a point cloud. Simulation particle data is 3D, time-dependent, vector attributes and the main focus of the paper is multifield visualization.

Jankun-Kelly and Mehta [JKM06] introduce a glyph based method for visualizing the nematic liquid crystal alignment tensor. Their method, communicate both the strength of the uniaxial alignment and the amount of biaxiality and, unlike previous methods it does not distort features of interest. Their glyph is inspired by the work of Kindlmann [Kin06] with a different parameterization of superelipsoids. Unlike previous work, their parameterization can represent negative uniaxial arrangements and also can represent real symmetric traceless tensors - real symmetric tensors whose eigenvalues sum to zero. 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. Based on work by Kindlmann [Kin06] but can represent negative uniaxial arrangements and real symmetric traceless tensors. The method described handles 3D, static data and the main challenge of the paper is multifield visualization.

Liquid crystal is an intermediate state between liquid and solid states, where molecules have lost most of their positional order but retain some orientational order. Rapid changes of orientation of liquid crystal molecules over space create defect structures. Mehta and Jankun-Kelly [MKJ06] present a method for semi-automatic detection and visualization of defects in unstructured models of nematic liquid crystals (NLC), a previously unsolved problem. Nematic liquid crystals (NLCs) are of interest to physicists as a simple and cost-effective sensor platform due to its high sensitivity to magnetic and electric fields (see Figure 11). Defect detection is based on total angular change of crystal orientation over a node neighborhood. There are two steps: first a preprocessing step builds a node connectivity list based on nearest neighbor paths [Cle79, HS03]. A second step computes the total angular rotation of a node by traversing its neighbors in the node connectivity list. Then a node is classified as a de-
6.3. Gravitation

Historically, this field has been placed within mechanics because of Newton’s contribution to both areas. His model accounts for the orbits of planets and the moon as well as for the movement of tides. 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 \[\text{[bru10g]}\].

We review papers that report on explanatory and illustrative visualization used to communicate theories of general and special relativity \[\text{[WBE’05]}\] and visualize physical aspects of the Gödel universe \[\text{[GB08, GMDW09]}\].

2005 saw the 100th anniversary of Einstein’s publications on special relativity, the photoelectric effect and Brownian motion. Communicating these theories to a wider audience requires a range of different methods. Weiskopf et al. \[\text{[WBE’05]}\] describe several examples of visualizations produced for this purpose, and also detail some techniques for image-based rendering of special relativity. For special relativistic rendering, the authors use a standard rendering pipeline with the Lorentz transformation forming an additional step. For general relativistic ray tracing, they extend an existing system to support manifolds defined by different charts, and finally they describe their process in creating a video of a journey from Earth through the solar system for an exhibition. The work on special relativity is also described in work by Weinberg \[\text{[Wer72]}\], and general relativistic ray tracing is implemented by extending work by Gröne \[\text{[Gro96]}\]. For the solar system journey, the short documentary film by R. Eames and C. Eames \[\text{[EE68]}\] and the work by Hanson et al. \[\text{[HFW00]}\] are cited as examples over similar time and length scales. The techniques presented process 3D, static data and the main challenge is learning and applying theories of general and special relativity.

Grave and Buser \[\text{[GB08]}\] visualize physical aspects of the Gödel universe, a theoretic universe which is a valid solution of Einstein’s field equations of general relativity. This work introduces two techniques to speed-up rendering of images in the Gödel universe and enable the application of a direct illumination model. The first technique uses preprocessing and lookup tables to allow recalculation of images at interactive frame rates, the second technique uses symmetries of Gödel space-time to reduce the problem size and necessary calculations. An overview of visualization of special and general relativity is found in work by Weiskopf et al. \[\text{[WBE’06]}\]. This the first work of its kind that visualizes the Gödel universe. Data processed is made of a 3D polyhedral model and the light paths in the Gödel’s universe. The techniques describe handle 3D, time-dependent, scalar on a unstructured grid. The main challenge of the paper is learning and using the physics required to do the simulation.

Grave et al. \[\text{[GMDW09]}\] visualize arbitrary geometry using local illumination in the Gödel’s universe at interactive rates. Grave et al. \[\text{[GMDW09]}\] derive the analytical solution for the propagation of light (geodesic equations) in Gödel’s universe. They use these equations to calculate the position on the image plane at which each triangle vertex is visible. They use isometric transformations to enable arbitrary observer positions and to apply local illumination models. Using graphics hardware they achieve interactive frame rates for visualizing arbitrary geometry using local illumination in the Gödel’s universe (see Figure 12). This work extends Grave and Buser \[\text{[GB08]}\] by allowing object movement and introducing non-interactive local illumination. Kajari et al. \[\text{[KWSD04]}\] found a set of coordinates for the Gödel universe, presented its symmetries and a special solution to the geodesic equations. Data processed consists of a 3D polyhedral model and the light paths in the Gödel’s universe. Data is 3D, time-dependent, scalar on a unstructured grid. The main challenge of the paper is learning and using the science required to do the simulation and the visualization.
6.4. 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 volumetric bodies with mass distribution in rigid-body dynamics. Elasticity is the mechanics of deformable solids, hydrostatic and hydrodynamics deal with fluids at rest and in motion [bri10g].

This section describes literature that visualize the turbulent mixing layer between two fluids [LBM*06] and structural mechanics simulations [BGG*06].

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

The Material Point Method is a method for structural mechanics simulations which represents solid materials using many individual particles. Bigler et al. [BGG*06] explain and evaluate two methods of augmenting the visualization of particle data using ambient occlusion and silhouette edges. Rendering of the Material Point Method Data is done using an interactive ray tracer [PPL*99]. Ambient occlusion [Ste03] is a shading model which enhances the perception of surfaces within a volume. This model incorporates diffuse illumination, which is attenuated by occlusions in the local vicinity of a surface point. Ambient occlusion values are precomputed as textures which are mapped to particles during rendering. Edges are discovered by convolving the image with a Laplacian. By using a threshold in the magnitude of the Laplacian, edges corresponding to different degrees of discontinuity can be selectively shown. These two methods are evaluated by the application scientists. While ambient occlusion improves perceptions, it requires memory for loading textures and thus it reduces the number of time steps of data that can be loaded in memory. Silhouetted edges help scientists to better see edges and shadowed regions. Bigler et al. use an interactive ray caster [PPL*99] to render Material Point Method Data. They apply Stewart’s shading model [Ste03] to particle shading and they use work by Saito and Takahashi [ST90] and McCool [McC00] to produce silhouette edges for objects in the scene. The authors evaluate both these methods as enhancements for Material Point Method Data visualizations. The system presented processes 3D, time-dependent, tensor, particle data. The main focus of the paper is to quantify the effectiveness of two methods of augmenting the visualization of particle data.

6.5. Optics

Optics studies behavior and properties of light. Geometrical optics deals with tracing of light rays and studies the formation of images by lenses, microscopes, telescopes and other optical devices. Physical optics deals with wave phenomena such as interference and diffraction [bri10g].

A paper that visualizes the optical power flow through a C-Shaped nano-aperture [SBH*04] is outlined.

The paper uses an abstract (simplified) visualization method to visualize specific features in the topology of the optical power flow over a C-shaped nano-aperture. The work develops from and utilizes the feature based topology visualization technique of the Helman and Hesselink [HH89, HH91]. The flows are characterized by analyzing particle paths (streamlines), which are classified into one of the following topologies: Degenerate repelling node, repelling star, repelling node, repelling focus, center, attracting focus, and attracting star. The paper describes the methods for identifying and marking the critical points through the topology mnemonic with critical points outgoing tangent lines being marked red with incoming tangents represented by yellow lines. One of the main areas of related work is that of topological vector

Figure 12: Multiply appearing objects and a point light source in the Gödel’s universe [GMDW09].
field [Mo90]. The techniques discussed process 3D, time-dependent, uniform resolution, regular grid, vector data. The paper is in the area of energy flow visualization and its main challenge is the science describing the phenomena presented.

7. Directions for Future Work and Conclusions

Based on our classification and discussions we identify the following directions for future work in visualization for the physical sciences. These directions complement the top visualization research problems of Johnson [Jo04].

- **Think about the science.** We note that most of the work has been in sound and general relativity visualization. We believe that close collaboration with physical scientists and understanding the science involved in a specific problem will result in new problems for the visualization community and in innovative solutions that will advance both visualization and the physical science involved.

- **Quantify effectiveness.** Very little work has been done comparing various visualization techniques for a specific domain of the physical sciences. We identify this as a direction for future work.

- **Represent error and uncertainty.** Only one paper deals with representing error and uncertainty. This remains a top direction for future research in visualization for the physical sciences.

- **Efficiently utilizing novel hardware architectures.** Most research on efficiently utilizing novel hardware architectures has been focused on chemistry. Research on how the GPUs would benefit the other physical sciences is a promising research direction.

- **Feature detection.** We believe feature detection and feature tracking are very relevant to the physical scientists and valuable contributions to this area are most successful when done in close collaboration with them.

- **Multifield visualization.** We believe realistic visualization of phenomena may be useful to a wide range of physical scientists so we think this is a good direction for future research.

- **Scalable, distributed and grid-based visualization.** Little work has been done in this area, and we believe there are ample opportunities for innovative research.

From the other top visualization problems proposed by Johnson [Jo04], we believe integrated problem solving environments and time dependent visualization are both relevant and good research directions for visualization in the physical sciences.

In this state-of-the-art report we have provided a comprehensive view on visualization solutions for the physical sciences developed in the last eight years. We started by providing an example of typical challenges faced by a physical scientist. We introduced a classification for the varied visualization solutions provided for physical sciences. This classification allows us to provide a much needed global view on 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 highlighting mature areas and suggest areas for future work. Through these collaborations, the visualization community can be exposed to new problems and can be asked to solve new challenges. In this way the visualization community can develop innovative techniques to solve our customers’ problems and keep the visualization field vibrant and relevant for the future.

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