Immersive Visual Analytics for Transformative Neutron Scattering Science

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Abstract

The ORNL Spallation Neutron Source (SNS) provides the most intense pulsed neutron beams in the world for scientific research and development across a broad range of disciplines. SNS experiments produce large volumes of complex data that are analyzed by scientists with varying degrees of experience using 3D visualization and analysis systems. However, it is notoriously difficult to achieve proficiency with 3D visualizations. Because 3D representations are key to understanding the neutron scattering data, scientists are unable to analyze their data in a timely fashion resulting in inefficient use of the limited and expensive SNS beam time. We believe a more intuitive interface for exploring neutron scattering data can be created by combining immersive virtual reality technology with high performance data analytics and human interaction. In this paper, we present our initial investigations of immersive visualization concepts as well as our vision for an immersive visual analytics framework that could lower the barriers to 3D exploratory data analysis of neutron scattering data at the SNS.

1 Introduction

In the early days of neutron scattering experiments, scientists manually configured instruments and recorded neutron counts by hand. Today scientists use sophisticated time-of-flight spectrometers to automatically collect hundreds of gigabytes of data in a matter of hours. As the size and dimensionality of the resulting data rapidly increase, scientists are realizing that they need new scalable techniques to glean insight from increasingly complex scientific data. In this paper, our team of visualization and neutron science researchers describe a potentially transformative vision of an immersive visual analytics framework that addresses the present and future data analysis challenges in materials science.

Over the last decade, numerous scientific visualization and analysis tools have emerged to help scientists explore large data sets. Given the physical nature of scientific data, three dimensional (3D) visualizations are the centerpiece of most advanced instances of such tools. The use of 3D visualization in these scenarios is justified

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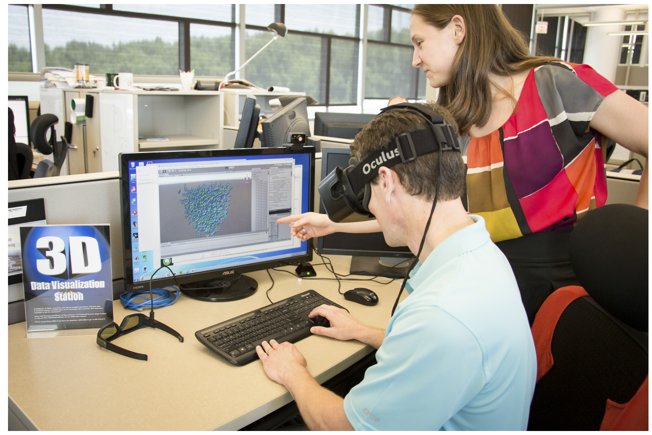

Figure 1: We developed a prototype Unity application as a proof-of-concept for virtual reality exploration of crystal structure data and neutron scattering data. This figure shows our demonstration of the resulting prototype at the Joint NSRC Workshop 2015: Big, Deep, and Smart Data Analytics in Materials Imaging.

since the representation provides an important affordance of material structures during analytical discourse and it enables perspectives at non-human scales [16]. Nevertheless, the learning curves for 3D visualization and analysis tools are notoriously steep due to complex user interfaces. Furthermore, virtual navigation of 3D environments is challenging with the standard mouse and keyboard interface [7]. For these reasons, we believe a new approach that facilitates more intuitive exploration of 3D visualizations is needed to unlock the full potential of scientific analysis.

The most attractive solution would be to automatically find scientific insights from the data using data analytics. However, the tasks are too exploratory for a completely automated solution. When an automated process is discovered, the goal of data visualization will shift from exploration to the confirmation and communication of results. For now, scientists mostly need exploratory systems that provide access to all the data and are not confined to the original hypothesis that prompted the experiment. Indeed, history has proven that the most significant discoveries are often unexpected (e.g., Pasteur's immunization principles, Columbus's discovery of America) [2]. On the other hand, a process entirely dependent on manual human investigations is also not feasible due to the volume and complexity of the data. Some automated data analytics are needed to guide the user and reduce the search space.

Given these constraints, we believe a visual analytics approach, combining the strengths of humans with the power of computational machines, is the most promising strategy for transforming scientific data analysis. Equally important, we must address the varying degrees of familiarity with analysis tools by providing highly interactive and intuitive systems that make sophisticated visual analysis procedures accessible.

More specifically, we have embraced a new approach that harnesses the power of virtual reality (VR) immersion within a visual

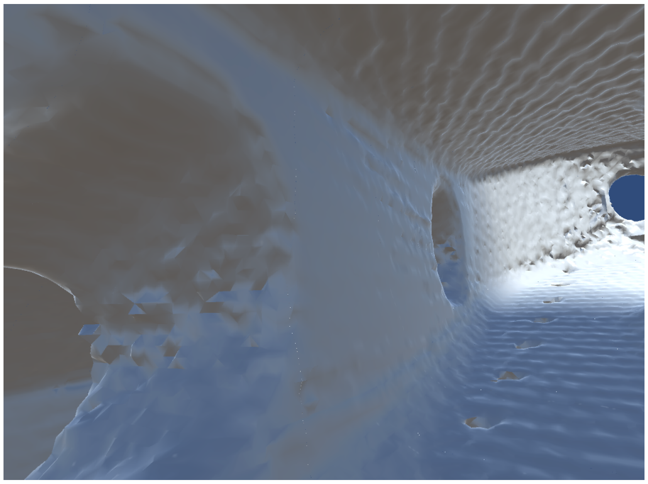

Figure 2: A 3D printed turbine blade was imaged using neutron tomography at ORNL's HFIR CG-1D imaging beamline for comparison against the original CAD model. To visualize the turbine blade with the Oculus Rift HMD, we created a simplified mesh by extracting isosurfaces from the scan point cloud data. In this figure, the view from inside the turbine is shown after navigating the space in our Unity-based prototype application. This unique perspective provides valuable insight on the accuracy of the 3D printing process.

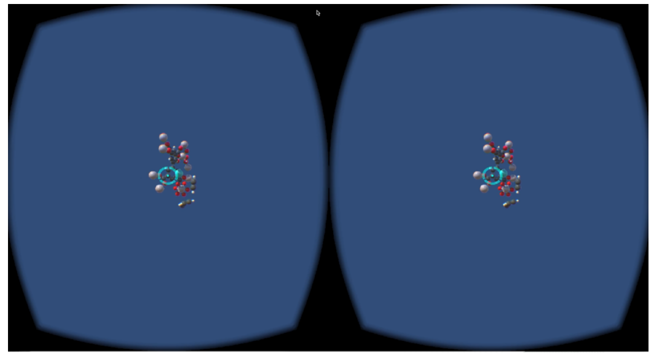

Figure 3: In our Oculus Rift HMD prototype, we used gaze interactions to select geometries in the 3D scene. In this figure, a crystal structure is visualized and crosshair rendering is enabled to help users target objects of interest and save locations.

analytics framework. We believe, and our early results confirm, that this strategy holds the potential to lower usability barriers and dramatically enhance knowledge discovery in neutron scattering and other similar scientific domains. New immersive technologies such as portable head mounted displays (HMDs) are flooding the consumer market. Furthermore, rapid technological advances are occurring with high resolution displays as well as equipment to track user interactions with these displays. The combination of affordability, acceptable performance, and straightforward development tools provides an ideal environment for innovation. Furthermore, as the technology is introduced to the general public, familiarity with VR and immersive interfaces increases, which reduces the learning curves for practical utilization in different scenarios.

In this paper, we describe our vision for an immersive visual analytics framework with illustrations targeting neutron scattering science. After providing background on data analysis challenges in neutron scattering, we introduce our initial investigations of immersive visualization using the Oculus Rift HMD and the Oak Ridge National Laboratory's (ORNL) interactive, stereoscopic display wall, called EVEREST. Then, we describe our vision for an immersive visual analytics framework, which is a multi-disciplinary effort that could enable scientists to ascend to new peaks in materials science.

2 Background

Facilities such as ORNL's Spallation Neutron Source (SNS) support users from all over the world with varying degrees of experience and technical analysis abilities. The visualization and analysis tools available to these users must provide an accessible user experience while maintaining the advanced capabilities needed to tackle important and challenging scientific questions. Timely visualization and analysis tools provide feedback for users, helping them make optimal use of limited and expensive SNS beam time.

Neutron scientists study materials with complex crystal structures that are described by large unit cells often containing tens to millions of atoms. These structures can be difficult to conceptualize in 2D visual representations. Furthermore, 2D projections hinder the identification of meaningful patterns or anomalies. Due to the physical nature of the data, 3D visualizations provide a more natural representation for data exploration.

Several visualization and analysis tools (e.g., Mantid, ParaView, and applications for the Interactive Data Language (IDL)) are maintained and supported by the SNS and its partner institutions. Despite the sophisticated capabilities of these tools, certain challenges remain. Visualization is a critical area for improvement. In fact, some users state that they "don't look at their data enough." Based on feedback from SNS scientists, user-friendliness and acceptable performance for large scale data are the two most important factors for adopting new technologies. Although the scientists who use modern materials science facilities like the SNS are extremely knowledgeable in growing materials and operating complicated neutron scattering and other related instruments, the majority of these scientists have limited proficiency with advanced visualization and visual analytics systems. To ensure scientists can practically use such tools to explore their data, intuitive user interfaces and low latency are necessary. A growing realization of these fundamental requirements motivates our study of new avenues for visual data exploration in materials science.

3 Immersive Visual Analysis using the Oculus Rift

Armed with an Oculus Rift head-mounted device (HMD) and SNS data sets, we recently studied the feasibility of an immersive visual analysis system for neutron scattering data. In this section, we provide an overview of the resulting prototype for context, but the reader is encouraged to study our prior work for details [8].

The project objective was to design a system that minimizes the steep learning curves and often cumbersome navigation procedures associated with traditional 3D visualization tools. These tools can require significant training time to achieve proficiency, which often limits the depth of analysis that is achievable while scientists are working at the SNS facility. Instead, most analysis is conducted after leaving the SNS facility, which precludes modifications to instrument parameters during the experiment. Having more accessible analysis tools will allow SNS users to more quickly understand their data and enjoy a more productive time period at the facility.

We hypothesized that the Oculus Rift HMD would provide more intuitive and natural navigation and interaction with the data, thereby increasing the efficiency of scientific analysis and reducing knowledge discovery timelines. In close collaboration with neutron scattering scientists, we developed a prototype using Blender [3] and the Unity game engine [15]. To minimize latency effects and field rapid iterations, we formulated a streamlined graphical model construction and optimization process. By leveraging the Unity development environment and its direct integration with the Oculus

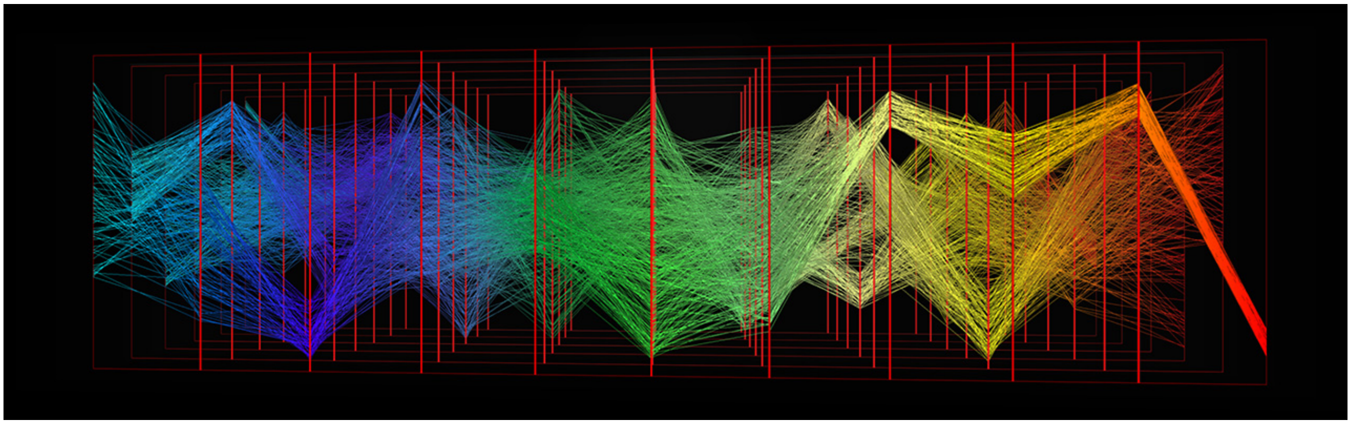

Figure 4: To capitalize on the stereoscopic 37 mega-pixel display wall in the ORNL EVEREST visualization laboratory and its human interactive tracking capabilities, we developed a stereoscopic parallel coordinates prototype application. The implementation uses the depth dimension to arrange multiple parallel coordinate plots. For example, the depth dimension can be mapped to time to allow temporal navigation. Additional interactions are envisioned to allow views from the right or left perspective in the 3D scene, as well as zoom and pan operations.

Rift, we quickly generated new iterations for informal evaluations with SNS scientists.

Our prototype ingested data from both crystal structure data and neutron imaging data. Using Blender and Atomic Blender [1], we created optimized meshes from the crystal structures for molecules consisting of up to 12,000 atoms. We also tested procedural mesh generation in Unity for molecules composed of up to 19,000 atoms. The volume of neutron imaging data and its point cloud representation was not well-suited to prototyping in Unity. To overcome this limitation, a custom volume rendering software was used to extract isosurfaces and create meshes from the volumetric data. In Figure 2, an example mesh is shown that was produced by applying the method to a large point cloud data set of a turbine blade. Generated using a large-scale 3D printer, the blade was scanned using neutron scattering instruments and compared to the original CAD model sent to the printer [17]. Prior to importing the data into Unity, we reduced the mesh to less than one million triangles. Although the prototype does not yet offer a direct connection to SNS instrument data streams, it demonstrates the potential for scientists to examine their data and refine experimental parameters within minutes of collection–a key goal of the SNS.

Beyond requiring efficient data processing, materials science analysis tools must be intuitively usable since they cater to such a variety of users. Our prototype supported interaction through game controllers (with keyboard and mouse as an alternative) and with gaze using Oculus head-tracking. Figure 1 shows a demonstration of an initial version of the prototype at the 2015 Joint NSRC Workshop on Big, Deep, and Smart Data Analytics in Materials Imaging, in which scientists could navigate and interact with crystal structure data. Figure 3 shows an example of the gaze interaction provided. The prototype tracked the center of the field of view and used ray casting to find intersections of scene geometries with the eye gaze vector. To assist object targeting, we provided an option to display a crosshair reticle during gaze targeting. Furthermore, the system allowed the user to save waypoints and target object locations in a scene. Location tracking support was added in anticipation of future remote virtual collaboration and 3D route reconstructions. At our demonstrations, the gaze interaction feature was intuitive to users, and only explanations of the buttons for entering and exiting target mode were required.

We informally evaluated our Oculus HMD prototype with several materials science researchers at scientific workshops, group meetings, and one-on-one demonstrations. In all cases, we received positive feedback on the potential of the approach to increase the efficiency of scientific analysis, especially for SNS facility users who were less proficient with 3D visualization tools. The prototype exhibited satisfactory performance, even for large models like the turbine blade, and controls were quickly understood by users. In particular, researchers commented on the ease of navigation through the data as compared to the difficulty with navigating 3D scenes using a standard workshop configuration. As we gathered feedback from these informal evaluations, we refined the prototype features and distributed new releases. In addition to feedback on the prototype functionality, the demonstrations often inspired the researchers to suggest alternative ways to employ immersive visualizations in materials science. Given the informal nature of our evaluations, we acknowledge that more formal user studies are needed to confirm our results. However, we believe these initial findings corroborate the notion that an immersive visual analysis system can transform knowledge discovery for materials science at the SNS.

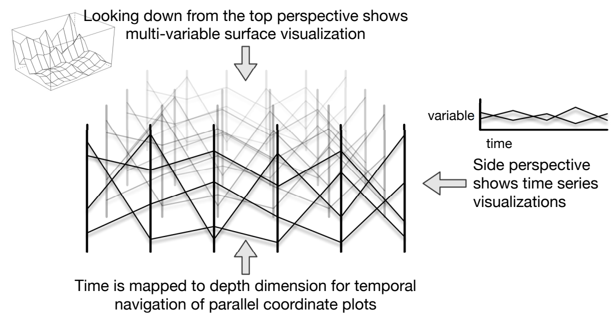

Figure 5: The stereoscopic parallel coordinates implementation provides a unique opportunity to explore different views of the data. If viewed head-on, the user will see multiple parallel coordinate plots that fade into the distance according to time. If viewed from the side, the view is morphed into a time series plot. From above, a surface plot can show both time and space mappings for a tuple or some summarization of tuples. In addition, zoom and pan operations are achievable from each perspective.

3.1 Immersive Information Visualization at EVEREST

The EVEREST visualization laboratory at ORNL features a stereoscopic 37 mega-pixel display wall. In addition, the display wall

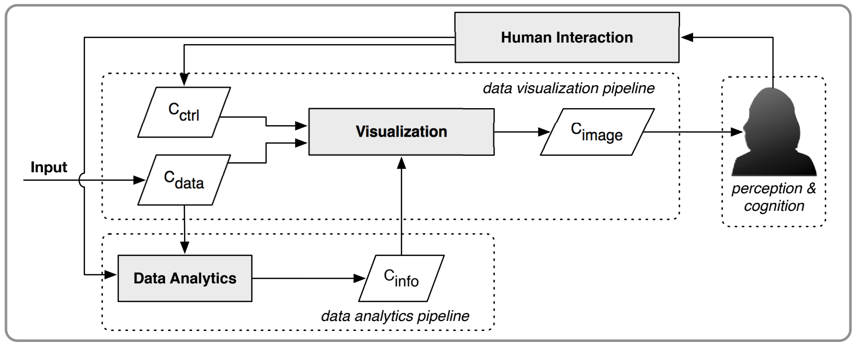

Figure 6: We formulated an immersive visual analytics framework drawing from our initial investigations with immersive visualization and our knowledge of the scientific needs for 3D visualization and analysis. The figure provides a notional view of the framework and extends the information-assisted visualization process introduced by Chen et al. [5]. The framework is centered on human interaction with data visualizations. The human is assisted by high performance rendering algorithms and an adaptive data analytics engine that capitalizes on human interactions with the display.

is coupled with a room level tracking system, which allows human interactions with the display. To investigate ways to leverage the unique capabilities of EVEREST for interactive analysis of complex data, we developed an OpenGL implementation of stereoscopic parallel coordinates (see Figure 4). Popularized by Inselberg [11], a parallel coordinates plot is a popular information visualization technique that transforms multivariate data into a 2D visualization without information loss. Working with a table of data, each vertical axis in parallel coordinates represents a column in the table and the axes are laid out in parallel horizontally. Then, each row tuple from the table is converted into a polyline by connecting normalized points placed on each axis.

We extended the parallel coordinates concept by utilizing a third dimension in the display to render stereoscopic parallel coordinates. For example, we can map time to the depth dimension and move forward or backward in time to explore the multivariate associations at different instants. The effect is similar to the user experience of the Apple Time Machine application for exploring backups of computer file systems. The time navigation is compelling in the EVEREST environment, but could also be applicable to an HMD experience.

As shown in Figure 5, we also formulated a new interaction capability for the stereoscopic parallel coordinates that would allow the user to select a set of axes and rotate the plot to reveal time series visualizations. The parallel coordinate axes would animate from the standard plot configuration to a view from the side, which rotates the depth dimension perpendicular to the viewer's gaze direction. Since the depth dimension is mapped to time, this rotation would produce a time series visualization of the selected variables. The action is reversible to rebuild the original parallel coordinates display. Furthermore, time range selections could be set in the time series view to constrain the data shown in the parallel coordinates plot. Likewise, range selections in the parallel coordinates plot could persist to highlight or filter the data depicted in the time series plots.

The stereoscopic parallel coordinates method would also permit a view from above. Here we envision the user selecting a polyline from each parallel coordinate plot in the depth dimension to build a surface plot. If multiple polylines are selected from each parallel coordinate plot, a statistical summary (e.g., mean, standard deviation) surface can be shown. We are currently implementing these views, and we believe the concept can be generalized to support other information visualization techniques.

4 A Vision for Immersive Visual Analytics for Transformative Materials Science

Based on both our initial immersive visualization endeavors and familiarity with the limitations of current visual analysis tools, we have formulated a vision of an immersive visual analytics framework for materials science. As shown in Figure 6, the proposed framework orchestrates human interactions, large scale data visualization, and data analytics into an exploratory analysis system that can be applied to scientific data. To be successful, the framework must leverage the latest immersive display technologies and high performance computing to allow intuitive interactions, multi-scale rendering, and adaptive data analytics. In the remainder of this section, we will discuss these key capabilities.

4.1 Intuitive Human Interactions

Since visual analytics is inherently a human-centered process, the success of an immersive visual analytics framework hinges upon the user's ability to intuitively interact with the underlying data behind the visualization. The user must be able to draw from their expertise and background knowledge to dynamically study the data and engage in the sensemaking process [12]. The sensemaking process consists of foraging and synthesis stages. In the foraging stage, the data are filtered and gathered to discover relevant information. The relevant information is then used for the synthesis stage, where hypotheses are formulated and confirmed. To maximize sensemaking capabilities, semantic interactions [9], which combine foraging and synthesis capabilities, should be integrated to the extent possible.

Our initial studies taught us that interactions within an immersive display can be a challenge. Handheld and tracking systems help replace the loss of the typical mouse and keyboard input devices and, in some cases, can be more intuitive. Gaze interactions are also available, which can be more natural but difficult to design. Regardless of the input method, the interactions provided by the framework must be directly embedded in the immersive display and utilize visual metaphors that can be quickly grasped by the user.

The framework must provide common interactions such as searching, highlighting, annotating, and rearranging elements. As connections between user interactions and data analytics are made, the complexities of the underlying statistical models should be hidden from the user to promote a seamless experience. During analysis, the framework will capture the user's interactions and feed the underlying statistical models in a supplemental analytics pipeline. The changes to the models will then be propagated to the display to augment the exploration process. These updates must be fast and reversible to maximize the user's ability to freely explore the data.

For example, if a data item is highlighted, the system should search for similar items. The resulting set of similar items could then be rendered in a more visually salient manner to bring these items to the user's attention. Due to the physical nature of the 3D environment, some of the similar items may be outside the field of view. When this situation occurs, arrows on the peripheral of the display could be shown to direct the user to the locations of interest.

Most scientists are not familiar with 3D visualization and analysis tools. Instead, they often use 2D visualization tools to explore the data and 3D visualizations are reserved for static images or movies to communicate results. To make 3D visualization and analysis more accessible, we must design interactions with the 3D scene in such a way that the essence of the more familiar 2D interactions are captured. For example, scientists will often use 2D planes to interactively slice a 3D volume of data. This process yields a 2D visualization through the 3D volume and the scientist can translate and rotate the plane to explore the data. We can capture the essence of the 2D plane slicing method by tracking the user's gaze and hand gestures while also providing the context of the overall 3D volume visualization using a semi-transparent rendering technique. By this method, the slices of data can be selected for analysis, annotation, and storage in a supplemental knowledge repository. If the supplemental 2D slice plots are displayed during this interactive process, the combination of 2D plots in an immersive 3D scene could produce user discomfort. To avoid such situations, it will be advantageous to design representations that are consistent with the virtual scene, but using interactions that maintain the essence of the more familiar 2D interactions.

Developing these VR interactions will require the translation of prior human-centered scientific analysis theories and the exploration of new fundamental ideas. In particular, research on Information-rich Virtual Environments (IRVEs) will be directly applicable. IRVEs are designed to enhance virtual environments that display spatial associations tied to the physical features of the data. By harnessing information visualization techniques, IRVEs visually encode additional information into 3D environments beyond the natural representations of the data's spatial properties. Bowman et al. describe potential applications and early research strategies in the area of IRVEs [4], and Polys et al. delve deeper into the depth and gestalt cues that affect analysis tasks within these environments [13]. Usability studies on IRVEs and other human-centered virtual environment designs will help identify features needed for immersive visualizations for scientific analysis.

4.2 Large Scale Data Visualizations with High Performance Computing

As the volume and complexity of scientific data continues to grow, the importance of high performance computing continues to dominate big data analysis. Without fast visualization and analysis algorithms, the volume of data far outpaces our ability to analyze it. Since latency is crucial to a favorable VR experience, the increasing power of high performance computing must be leveraged to maximize responsiveness, especially while analyzing raw data as it is collected from high velocity instrument streams.

With neutron scattering, the data are often visualized as point clouds, isosurfaces, or volume visualizations. For these data we can leverage decades of computer graphics research to implement level-of-detail rendering with optimized indexing and aggregation schemes that limit the number of graphical primitives rendered based on the virtual proximity of user's viewpoint [6]. The proposed framework must also take advantage of the rendering optimization schemes proposed for computer games, simulations, and scientific visualization to reduce latency and increase increase the realism of the immersive experience. Furthermore, fast geometrical indexing schemes are required to quickly identify data items selected with the interaction techniques.

In addition, we believe distributed rendering and analytical processing can be harnessed so that the display system is not burdened with the full rendering workflow. For example, we are developing software infrastructure to remotely render extremely large scale scientific data using GPUs on the Titan supercomputer in the Oak Ridge Leadership Computing Facility (OLCF). Meanwhile, we can increase the number of pixels available for displaying the data by using a high resolution display, such as the 37 mega-pixel display wall in the ORNL EVEREST visualization laboratory. Besides its high resolution stereoscopic displays, EVEREST includes a high performance tracking system that captures human gestures. The tracking system can be used to enable natural interactions with the high resolution display. Smaller scale GPU clusters are envisioned at scientific data analysis facilities to allow interactive exploratory investigations at the location where the data is generated.

4.3 Smart Immersive Data Analytics

In conjunction with intuitive interactions and high performance computing components, we can capture human feedback to feed real-time machine learning algorithms that learn from the user's interactions and adapt the visualizations. Often called intelligent user interfaces, such systems leverage human interactions to label data, infer importance using multiple feature spaces, and ultimately feed the construction of a model to predict what is of interest to the user. An online recommender system can then be leveraged to highlight or filter potentially important associations and data items. For example, we can make the potentially important associations that are found with the machine learning algorithms more visually salient using pre-attentive processing guidelines from perceptual psychology [10]. For large, complex data sets where manual inspection is challenging, this approach can be a game-changer as it lets the user focus on the most interesting data, which are defined by the user during the analysis session.

We envision an immersive experience that is similar to our visual text analytics system, called Gryffin. Gryffin is a search-based document analysis system that displays 2D information visualizations of search hits for large document collections [14]. When a keyword search is executed, the search results are shown as a list of document summaries. Typically, the user must manually study each search hit to ensure all relevant documents are discovered. With a large list, it is not feasible to visit every document and some relevant documents may be missed. Using Gryffin's interface, the user can interactively explore the search results and mark documents as relevant or irrelevant based a topic of interest. These interactions are then used behind the scenes to label the documents. The labels are subsequently passed to a machine learning algorithm to construct a model of relevant items. This model is then used to predict the relevance of the unlabeled documents and the list is rearranged so that potentially relevant documents are moved to the top of the list and vice versa. In a very large list of search results, the user can concentrate on a small portion of the list to effectively find interesting documents.

We believe a similar effect can be achieved in an immersive VR display. In our Oculus prototype, we tested this idea by capturing the user's gaze to highlight geometries of interest. If the user focuses the gaze for an extended period of time, the object is highlighted and saved. In conjunction with gestural inputs, this method can be used to label an item as relevant in the display. Variations to the interaction can be used to label other items irrelevant. The two classes of items, relevant and irrelevant, can then be used to predict the relevance of the remaining unlabeled elements. Through visual cues, the system could then highlight the potentially relevant items or, conversely, hide the potentially irrelevant items.

Given the volume and complexity of data, a machine-guided analysis system is the most viable solution. By leveraging both automated analytics and human-centered analysis, the resulting system can tackle challenges neither could solve easily in isolation. By hiding irrelevant items, the approach could improve latency. Furthermore, the system could maintain a knowledge repository storing labels, algorithmic predictions, annotations, and discoveries. Building a knowledge repository from expert users' interactions with the system could provide guidance to novice users and help initiate new data analysis sessions based on similarities with prior work. In addition, the serialization of user interactions during the analysis session will provide provenance information. This interaction history will promote reproducibility of knowledge discovery, collaborative sharing with other users, and communication of results.

4.4 Multi-disciplinary Participatory Design

As immersive display technologies enjoy a surge in utilization, projects that apply immersive analytics in scientific domains should make conscious efforts to increase adoption rates and ensure proper responses to real-world data analysis challenges. We believe the best way to accomplish this goal is to include domain experts in the design, development, and evaluation stages. Indeed, we attribute the success of our initial efforts to close collaborations with neutron scattering experts. When domain experts are successfully integrated as a part of the team, the results respond to their actual needs, they are eager to adopt the concepts in routine workflows, and they will promote the ideas among their peers. Other practical considerations for participatory design strategies include modeling new interactions after current practices, connecting prototype implementations to scientific domains with pressing real-world challenges, and designs that orchestrate both human and computer strengths. Another goal should be the communication of results and training information for domain scientists. Such endeavors are vital to bridging the gap between the latest visualization advances and practical scientific analysis techniques.

To validate new systems, the tools must be evaluated using metrics and studies that are accepted in both the scientific domain as well as the Human-Computer Interaction (HCI) and visualization fields. In the latter, human subject studies and newer longitudinal studies are the standard approach for validating new techniques. However, in the scientific domains, a greater emphasis is placed on different metrics such as reduced knowledge discovery timelines, use cases that reveal new discoveries enabled by the new approach, and adoption rates among domain experts. In order to allow for cross-pollination of ideas, the visualization and HCI communities should recognize the importance of the evaluation metrics from scientific domains and give them equal treatment. Likewise, the results of more traditional HCI studies should be published in scientific venues in an accessible manner to educate future users.

5 Conclusion

At SNS, neutron scattering scientists need more intuitive 3D visualization and analysis tools that provide accessible interactions with large and complex data. Other scientific domains, such as climate and manufacturing, have similar challenges that 3D visualizations could alleviate. We believe immersive technology, such as the Oculus Rift HMD and the ORNL EVEREST stereoscopic display wall represent a viable path toward unlocking the full potential of large and complex scientific data.

Our initial endeavors and practical experience with materials scientists contribute to the evolution of our vision for immersive visual analytics. As we develop the framework, we will continue soliciting feedback from scientists in real-world projects and eventually conduct more formal evaluations of the resulting system. By orchestrating the strengths of humans and computers, especially high performance systems such as Titan, a successful visual analytics framework that capitalizes on the immersive experience could enable adaptive exploratory analysis and reduced knowledge discovery timelines–key requirements in the SNS mission to streamline user experiences both now and in the future.

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