

# Immersive Visualization for Materials Science Data Analysis using the Oculus Rift

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**Abstract**—In this paper, we propose strategies and objectives for immersive data visualization with applications in materials science using the Oculus Rift virtual reality headset. We provide background on currently available analysis tools for neutron scattering data and other large-scale materials science projects. In the context of the current challenges facing scientists, we discuss immersive virtual reality visualization as a potentially powerful solution. We introduce a prototype immersive visualization system, developed in conjunction with materials scientists at the Spallation Neutron Source, which we have used to explore large crystal structures and neutron scattering data. Finally, we offer our perspective on the greatest challenges that must be addressed to build effective and intuitive virtual reality analysis tools that will be useful for scientists in a wide range of fields.

## I. INTRODUCTION

In this work, we introduce an immersive visualization environment for materials science data and discuss general strategies for virtual reality applications in scientific research. Using an Oculus Rift head-mounted device (HMD), we demonstrate exploratory visualizations of crystal structure and neutron scattering data sets. Currently, researchers have access to powerful three dimensional (3D) visualization tools, including VMD [1], Mantid [2], and ParaView [3], allowing them to interactively explore large, complex scientific data and generate illuminating figures for communicating insight gleaned. However, these tools have steep learning curves for standard usage, and navigation of the data is difficult, even for advanced users. Moreover, most views are limited to two dimensional (2D) projections. The Oculus Rift<sup>1</sup> integrates immersive 3D rendering with predictive head tracking [4], [5] to provide intuitive comprehension and interaction with the data. In this project, our objective is to lower the barriers to entry for exploratory analysis of complex scientific data by leveraging

the Oculus Rift to provide intuitive interactions and efficient navigation in an immersive 3D environment.

This endeavor has been a collaborative effort with materials science experts as co-designers of the prototype system. We describe our initial results toward integrating the Oculus Rift into existing visualization tools, and we address issues that may affect the broader implementation of virtual reality immersive visualizations. Thus far, our experiments have encompassed virtual navigation of crystal structure data and exploration of a 3D-printed turbine blade imaged using the CG-1D Cold Neutron Imaging Facility<sup>2</sup> of the High Flux Isotope Reactor at Oak Ridge National Laboratory (ORNL). We include gaze interaction to “bookmark” points of interest in the data. We anticipate that these tools will assist researchers in rapid data exploration and help them acquire near real-time feedback for ongoing experiments. We also expect that the immersive visualizations accessible through the Oculus Rift will facilitate collaborative investigation of complex data sets and allow for the convenient sharing of knowledge.

Beyond introducing our approach for immersive visualization, we identify key research questions and propose strategies toward further development of virtual reality (VR) tools for scientific visualization and analysis. We suggest factors to consider when designing VR systems for scientific analysis purposes. We also pinpoint some of the key challenges that must be addressed to enable safe, comfortable, and intuitive experiences for diverse users. Finally, we address the human-centered strategies that are necessary to discover the most useful interfaces and interactions for analysis tasks. Using a human-centered approach, we can leverage scientists’ a priori knowledge and analysis procedures with innovative representations and machine learning tools to gain greater insight more efficiently than prior systems have allowed.

## II. RELATED WORK

Although much of the excitement about consumer level VR centers on video game development, many scientific and engineering applications for immersive visualizations have

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<sup>1</sup>Information about the Oculus Rift is available online at <https://www.oculus.com/en-us/rift/>.

<sup>2</sup>More information about the facility is available at <https://neutrons.ornl.gov/imaging>.

been explored. Medicine is one of the most extensively studied areas for scientific visualization using VR. Richard Satava has outlined several of the early uses of VR systems in medical training and surgical pre-planning [6]. He describes how surgeons have used VR models to practice and prepare for tendon transplants, surgical correction of facial bone deformities, plastic surgery procedures, and radiation therapy for tumors. An augmented reality system that fuses MRI scans with real-time video from neurosurgery is also presented, as well as surgical simulators for laparoscopic and abdominal procedures. Van Dam et al. detail similar applications and argue that VR offers substantial advantages for nonhuman-scale visualization, particularly for data that should be explored in multiple time and space scales [7]. These functions are especially challenging for user interface design, the authors point out, but VR has the potential to display a larger quantity of meaningful data and facilitate more natural interaction than traditional 2D visualization techniques.

Extensive research has been conducted regarding the perceptual mechanisms and analysis task strategies that affect how pattern-finding and analysis are performed in 3D, as opposed to 2D. Colin Ware points out that “the most powerful pattern-finding mechanisms of the brain work in 2D, not 3D” [8, p. 239]. Nevertheless, Ware argues that 3D user interfaces are likely to predominate in the long run, since humans are accustomed to perceiving, interacting with, and forming intuition about objects in a 3D world [8, p. 290]. A study by Cockburn and McKenzie in 2002 indicated that 3D interfaces for document retrieval tasks hindered user performance [9]. It should be noted that the virtual 3D environment in the Cockburn-McKenzie study was a 2D projection of a 3D environment. However, regardless of the results with virtual environments, users in this study sorted and retrieved documents more quickly in a physical 2D environment than in a physical 3D environment. This study demonstrates that 3D environments are not inherently better suited to analysis than 2D environments, underscoring the need for human-centered design. When building 3D immersive visualizations, researchers should carefully consider if a 3D VR environment is the most appropriate for a given task, and if so, which interactions should be implemented to best facilitate the analysis needs for that particular task.

Safety and usability should also be critically examined when designing VR applications. Davis et al. present a survey of research on cybersickness, whose symptoms constitute some of the most pressing safety concerns for VR [10]. In their review, the authors address risk factors for cybersickness with respect to individual users, VR devices, and tasks performed in VR. They also summarize mechanisms for assessing the severity of cybersickness symptoms, including physiological studies and self-reporting through questionnaires, and they propose strategies for mitigating the risks and severity of symptoms. Marks et al. highlight the importance of developing metrics to systematically assess latency, one of the most significant factors contributing to cybersickness symptoms [11]. Bowman et al. discuss mechanisms for the evaluation of both

user comfort and overall usability [12]. They examine how traditional methods for 2D User interface/User Experience usability evaluation may be applied to VR interfaces. They also discuss subjective measures that should be used to assess VR applications, including user comfort and ease of use.

### III. BACKGROUND

One of the most important barriers between performing an experiment and publishing the results is the complex and time-consuming effort that individual researchers apply to data reduction, visualization and analysis. While the first neutron scatterers had to manually set up their instrument and record neutron counts in handwriting a single point at a time, users at a modern time of flight spectrometer rapidly collect hundreds of gigabytes of data in less than one day. Rapid reduction, analysis, and visualization provide feedback for users, helping them make optimal use of limited beam time. Traditional line plots and cuts become less effective for rapid exploration of large multidimensional datasets.

Software must also be accessible to and customizable by users with a broad range of abilities and interests in programming. Facilities such as ORNL’s Spallation Neutron Source (SNS) support users with widely different levels of experience and technical ability. Visualization and analysis software suites must accommodate this range of users while maintaining the capabilities to address important and challenging scientific questions.

Addressing today’s scientific questions requires the study of materials with large, complex crystal structures. These materials are described by large unit cells regularly containing tens to millions of atoms. Given such large structures, 2D projections severely hinder users’ ability to conceptualize the structures and to identify meaningful patterns or anomalies.

The scattering function  $S(\mathbf{Q}, \omega)$  is often visualized using the software DAVE MSlice [13] and Horace [14], both of which are written in Interactive Data Language (IDL). While adequate for the facilities and instruments that existed when they were initially developed, these legacy tools struggle to scale up to data generated by new instruments at current facilities. The Mantid Project [2] was started in 2007 at ISIS<sup>3</sup>, partially in response to the need for an integrated, maintainable, and high performance solution.

Mantid utilizes the multidimensional visualization capabilities of ParaView. A custom application called the Vates Simple Interface and a variety of plugins for the ParaView application come bundled with Mantid. Challenges include navigating science requirements such as displaying the nonorthogonal basis vectors that describe complex crystal structures with a general purpose library expecting Cartesian coordinates. Many of the improvements are evolutionary instead of revolutionary. Interfaces are often derived from legacy software, with improvements including tight integration with Mantid’s data reduction algorithms and higher performance.

<sup>3</sup>ISIS is a pulsed neutron and muon source at the Rutherford Appleton Laboratory in Oxfordshire. More information is available at <http://www.isis.stfc.ac.uk/about/aboutisis.html>.

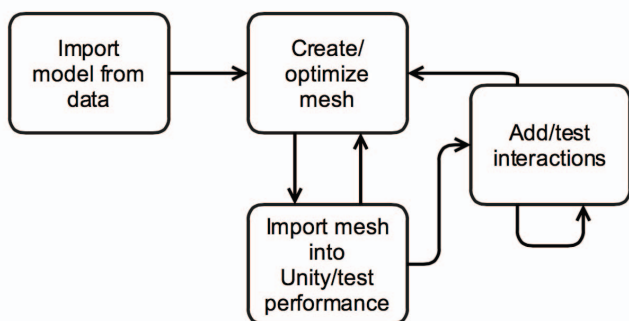


Fig. 1. Workflow for prototype immersive visualization environment.

Even though SNS, along with its partner institutions, maintains and provides support for Mantid and other analysis tools, challenges remain. Visualization is a particularly salient area of need, as evidenced by some users acknowledging that they “don’t look at their data enough.” Based on our observations and feedback from facility users, the two determining factors in the adoption of new technologies are user-friendliness and performance and scalability for big data. The scientists who make use of specialized materials science facilities are experts in growing materials and in the operation of neutron scattering, electron microscopy, or other appropriate instrumentation. The majority of these users have limited experience with visualization and visual analytics tools. In order for them to use such tools to gain insight about their data, the tools must have sufficiently intuitive controls and minimal latency.

The development of our immersive visualization tool has been motivated by the need for intuitive controls in an exploratory environment. Using a human-centered approach to design, we also aim for the tools to take advantage of users’ a priori knowledge and analysis strategies. To encourage adoption of new analysis tools, we must minimize the learning curve for effective usage while leveraging Mantid’s performance and specialized capabilities. We also anticipate that availability of meaningful visualization tools for materials science data will promote the sharing of knowledge in the field. These objectives have guided our approach to development of VR tools for data visualization.

#### IV. APPROACH

Materials science data continues to proliferate rapidly as the discipline grows and intersects with other fields. Due to the diversity of scientists and applications, many of the analysis techniques for materials science data are highly specialized. Analysis tools such as VMD, Mantid, and ParaView offer sophisticated features, but require significant training time for proficiency. Rather than taking advantage of these tools at the SNS user facilities, most scientists utilizing the instruments opt to analyze their data after returning to their home institutions. Consequently, their analysis cannot be used to guide their experimental controls. Our objective is to provide human-centered analysis tools that visiting researchers can utilize

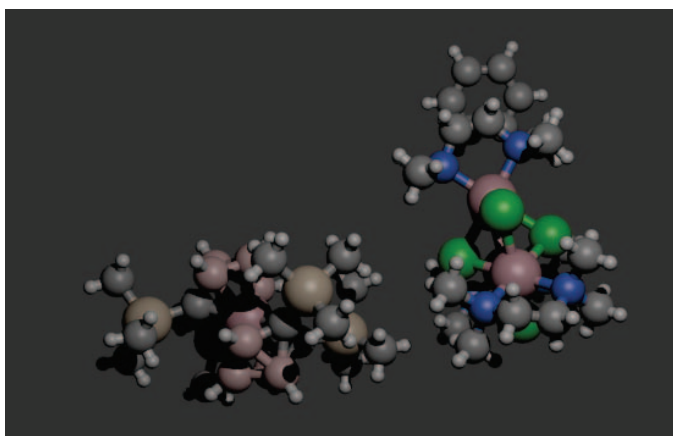
to immediately strengthen their understanding of their data. Ideally, scientists will be able to use the additional insight to ensure that their experiments are as productive and enlightening as possible.

For our applications in material science, our primary objective is to provide users intuitive means for exploring their data in near real-time. As a proof of concept, we built our prototype immersive visualization for Oculus Rift using Blender modeling software [15] and the Unity game engine [16]. An outline of the development workflow is shown in Figure 1. In order to ensure low latency and provide feedback on the data as quickly as possible, we prioritized the formulation of a streamlined process for model creation and optimization. Models can be imported, optimized, and exported to formats compatible with Unity in minutes. We leveraged Unity’s simplified development environment and built-in virtual reality integration to rapidly implement and test various interactions.

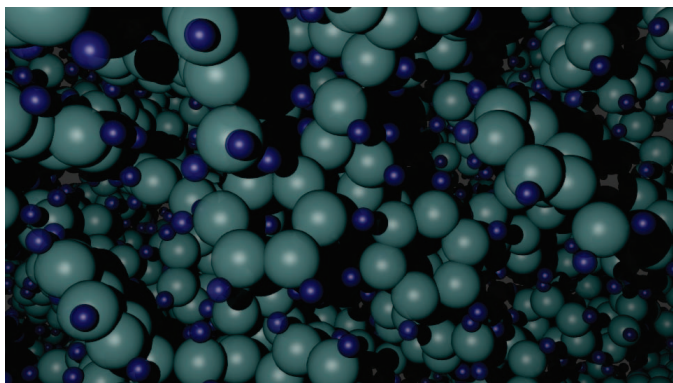
We imported crystal structure data from PDB and CIF formats, as well as neutron imaging data from VTK format. Using Blender and Atomic Blender [17], we created, experimented with, and optimized meshes from the crystal structures for molecules consisting of up to 12,000 atoms. We also tested procedural mesh generation in Unity for molecules composed of up to 19,000 atoms. The Blender model imported with Atomic Blender in NURBS format and exported as an FBX object achieved the best synthesis of appearance and low latency, consistently performing at 30 fps. Figure 2 shows renderings from models created using this technique.

Data from neutron imaging instruments proved more of a challenge for modeling and optimization. The volume of neutron scattering data was significantly larger, and its volumetric point cloud representation was not well-suited to prototyping in Unity. We relied on custom volume rendering software to extract isosurfaces and create meshes from the volume data, which could then be reduced and optimized. The turbine blade shown in Figure 3 is an example of a mesh produced using this method. This turbine blade was created using 3D-printing, then analyzed with neutron scattering to determine how closely the final product fit the original CAD model [18]. The extracted mesh depicted in Figure 3 was reduced to under one million triangles for import into Unity. Though our proof of concept technique does not yet offer near real-time feedback, it would enable researchers to view their data within minutes, so the knowledge gained could help refine experiments as they are carried out, offering a substantial improvement over current timelines for analysis.

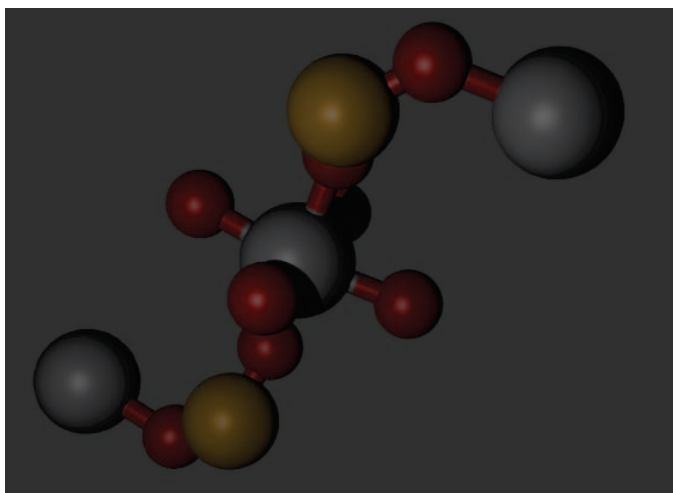
Coupled with timely feedback, intuitive interaction is the most critical need for materials science data analysis tools. Natural controls are particularly crucial in virtual reality environments where input may be limited. Oculus does not currently provide native hand tracking, but the Oculus Touch is slated to be released in the first half of 2016 [19]. We did not implement hand tracking, but mapped our navigation controls through Unity’s cross platform input manager. The cross platform input manager maps Xbox and other standard game controllers, but it allows for keyboard and mouse input as



(a) Structure of C<sub>37</sub> H<sub>95</sub> B<sub>8</sub> Cl<sub>5</sub> Co<sub>4</sub> N<sub>6</sub> Si<sub>4</sub>, modeled and rendered in Blender.



(b) Structure of styrene toluene, modeled and rendered in Blender.



(c) Structure for a sample Metal-organic Framework, modeled and rendered in Blender.

Fig. 2. Crystal structure data modeled using Blender. We utilized Atomic Blender to import PDB models, and we experimented with optimization of both NURBS and meshes to determine the best performing models for import into Unity.



Fig. 3. Mesh created by extracting isosurfaces from volumetric neutron scattering data of turbine blade. Custom software was used to extract and reduce the number of polygons in the mesh.



Fig. 4. Demonstration of virtual reality exploration of crystal structure data at the Joint NSRC Workshop 2015: Big, Deep, and Smart Data Analytics in Materials Imaging.

an alternative. At our demonstrations, we observed that many users had difficulty interacting with keyboard and mouse when they could not see their hands, but most users were able to use the Xbox controller intuitively. Figure 4 shows a demonstration of the first implementation of the prototype from the 2015 Joint NSRC Workshop on Big, Deep, and Smart Data Analytics in Materials Imaging. Users were able to “fly” through the data and, using the Oculus head-tracking, look around and view the data from different perspectives.

Our immersive visualization also incorporates gaze interaction, arguably the most natural form of interaction in virtual reality environments. Since one of our objectives is to support

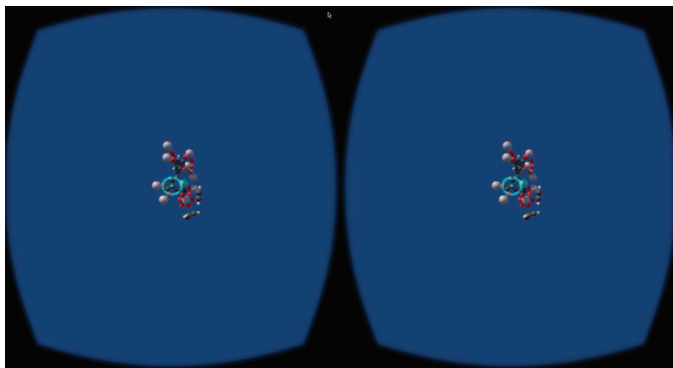


Fig. 5. Oculus Rift display with gaze interaction for crystal structure data. Since Oculus does not currently support eye tracking, crosshairs are used to help users target data points of interest and save locations.

remote virtual collaboration, we focused on allowing users to “bookmark” locations and data objects as an annotation that allows other users to take the same “journey” through the data. Oculus does not support eye tracking, so gaze interaction is accomplished by tracking the center anchor of the Oculus field of view and using raycasting to determine whether any data objects are encountered in that direction. In order to help users target objects more effectively, we provide a crosshair reticle that is rendered visible when a button is pressed to enter “target mode.” When the button to exit target mode is pressed, the reticle is no longer rendered. While in target mode, a user may save the current location of the avatar—including position and orientation—using a trigger button. If, when the trigger button is pressed, the reticle is targeting a data object, the trigger also bookmarks that data object and highlights it in a contrast color. When the trigger button is pressed, the user’s location is saved regardless of whether or not a data object is bookmarked. As an alternative, a user may bookmark a data object and simultaneously save location using “extended gaze” by focusing the reticle on the object of interest for longer than the specified gaze period (two seconds by default). A screenshot of the gaze interaction is shown in Figure 5. 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.

Our prototype immersive visualization has been well received by materials scientists at ORNL. The performance has been satisfactory, even for large models, and the controls were intuitive. Researchers have been particularly impressed by the ease of navigation through the data, since navigation through 3D data tends to be onerous when using 2D monitors. We iterated several features of our design based on feedback from demonstrations, and we received numerous suggestions for alternative uses of immersive visualizations in materials science.

In addition to developing the prototype tool using the Unity game engine, we are collaborating with software engineers and developers of specialized visualization tools towards the creation of more scalable and usable long-term solutions.

Developers of specialized visualization software used by SNS are working to integrate support for the Oculus Rift into their standard interface, and we have collaborated with them on guiding principles for interactions in VR. Together with a software engineering group at ORNL, we are also working to integrate our prototype and other VR visualizations into standard workflow tools used for scientific research.

## V. VIRTUAL REALITY FOR SCIENTIFIC VISUALIZATION

### A. Why now?

Enthusiasm for VR has risen and fallen several times in recent decades. Will the current wave, like previous ones, dissipate without sustainable and widely usable VR tools? Although there are no guarantees, we believe the current surge of interest will endure primarily because both VR hardware and software are now more accessible. Current head-mounted devices (HMDs) are more portable and affordable than CAVE environments or HMDs of the past, making them ideal tools for exploratory visualization. This factor is unique to the current movement and could result in the widespread utilization and democratization of VR technology.

The concept of a stereoscopic HMD was demonstrated at least as early as Ivan Sutherland’s device in 1965 [20]. After decades of iterative development, the Oculus Rift is the first HMD to deliver satisfactory VR performance on commodity hardware. Moreover, the API provided by Oculus, as well as the integration packages for commonly used video game engines, have removed many of the complexities of software development for VR. Since the release of the first Oculus prototype, several more HMD systems have been released, including the most affordable model, Google’s Cardboard VR [21].

The confluence of affordability, acceptable performance, and straightforward development tools has created an ideal climate for innovation. These factors have encouraged intensive development by competing hardware manufacturers, experienced video game designers, and casual enthusiasts. A favorable corollary to the accessibility of HMD hardware and development tools is the increased familiarity that the technology attains with the general public. As the technology is introduced to more people, familiarity with VR interfaces expands, which in turn, reduces the learning curve for the use of HMDs and further lowers the barriers to entry for development. All of these considerations have influenced our approach to immersive visualization for scientific analysis. The data visualization community should take advantage of the feedback available from this broad base of new VR users and developers. Our application in particular stands to benefit from this insight, since it targets users from various technical and scientific backgrounds.

### B. Challenges and Design Strategies

Over the course of our investigation, we have demonstrated the prototype to numerous scientists. In some cases, these encounters were one-time events, but with two materials science experts (who are also co-authors on this paper), the

testing occurred on a bi-weekly basis. By observing the scientists' reactions, collecting feedback, and capturing our own observations, we have identified several key challenges for bringing new VR systems to bear for scientific visualization. In the remainder of this section, we describe these challenges and discuss our design strategies.

1) *Safety, Comfort, and Ease of Use*: The first and perhaps most critical factors we considered were safety, comfort, and ease of use. Prompted by health warning screens on Oculus applications and in the development kit's documentation, we studied ways to mitigate adverse effects as we designed natural interactions in VR. Cybersickness is a significant limitation of the Oculus Rift system. The product documentation recommends no more than 30 minutes of uninterrupted use and suggests 15 minutes for new users. Cybersickness is not a new phenomenon [10], and best practices based on user studies are promoted to avoid it. However, beyond the immediate symptoms of cybersickness, questions remain as to the persisting short- and long-term effects. For example, we received reports of delayed dizziness from some scientists up to an hour after brief exploration of a 3D mesh using the Oculus Rift. Furthermore, co-authors of this paper have experienced nausea that lasted over 24 hours after prolonged use of a room-level stereoscopic display wall during development testing. Given the potential for more widespread use with current VR equipment, we believe more studies are needed to carefully investigate potential health and safety issues. Specifically, these studies should address the most effective ways to mitigate adverse effects and metrics to quantify whether a particular application is sufficiently safe for a particular user.

Another important safety issue is physical safety of the location where the Oculus device is operated. As the user will be unable to see the real world surroundings, the area must be open and clear of hazards. Furthermore, as the Oculus system recommends, the user should be seated during device operation, and an observer/spotter should be present to monitor the user—particularly for new users.

In our investigation we noted that latency has a significant effect on the user experience. When rendering lags, user discomfort rapidly increases, which degrades performance and, ultimately adoption potential. In the context of big data, the latency effect will be a key challenge to overcome. The most viable strategy to overcome latency is through optimized rendering algorithms and multi-scale representations running on powerful graphics hardware. In addition to minimizing latency, Michael Abrash has outlined the other hardware factors that must be addressed to avoid cybersickness risks [22]. He describes the need for each of the following:

- Wide field of view
- Sufficient resolution
- Low pixel persistence
- High refresh rate
- Displays illuminating all pixels simultaneously (global display)
- Excellent optics and capabilities for optical calibration
- Precise tracking

- Minimal latency

Abrash asserts that all of these factors are critical for offering users a sense of presence and that subpar performance for any of them could cause cybersickness. He also enumerates minimum specifications for each factor that, according to research at Valve, provide adequate VR performance.

2) *Adaptive and Intuitive Interactions*: Human interactions with the 3D environment should be both adaptive and intuitive to minimize cognitive burdens on the user. It is important to understand what interactive capabilities are important for each scientific use case to increase the usability of the system and stimulate the adoption in scientific analysis scenarios. One way to improve usability is through less intrusive, longitudinal studies (e.g., interviews, diaries, paired analysis sessions) of the traditional ways scientists interact with their data. Also, as with any multi-disciplinary problem, we believe domain scientists should be tightly integrated in the design team. As co-designers, they can directly use their domain knowledge and experience to shape the resulting system in meaningful ways, which could escalate both adoption rates and overall effectiveness of the resulting systems in the context of real-world problems in data-rich domains.

In the case of scientific analysis, the transition to a 3D environment can be difficult, as most scientists typically explore their data using 2D visualizations, and they have been doing so for decades. Careful thought should be devoted to ways to capture the essence of the most effective 2D interactions and bring them to bear in a 3D display. For instance, scientists will often slice 3D volume data using 2D plane slices. How might we allow the scientist to intuitively slice a 3D volume and visualize the result in a way that captures the immersive experience? We envision a 2D slicing plane widget that can be controlled by the user's gaze and hand gestures while providing the context of the overall 3D volume with a semi-transparent volume rendering. Slices could be intuitively selected and grabbed to analyze, annotate, and save for later use in a supporting knowledge repository. If the user is also presented with supplemental 2D plots in the viewer's peripheral area, will the display produce user discomfort or increased efficiency? If it is the former, it could be advantageous to devise representations that are consistent with the virtual world in which the user is immersed, but with interactions that capture the essence of established 2D interactions.

We believe the answers to these and other questions related to VR interaction for scientific analysis will be answered through studies of human-centered scientific analysis. The resulting theories will inform the development of new interactive VR prototypes that can be further studied for practical use. Likewise, studies of these prototypes will then contribute to new design iterations that will lead to more relevant and useful systems. Some of the research in this area focuses on Information-rich Virtual Environments (IRVEs), which enhance virtual environments created to display data whose spatial relationships are tied to physical features of the data. These virtual environments leverage information visualization

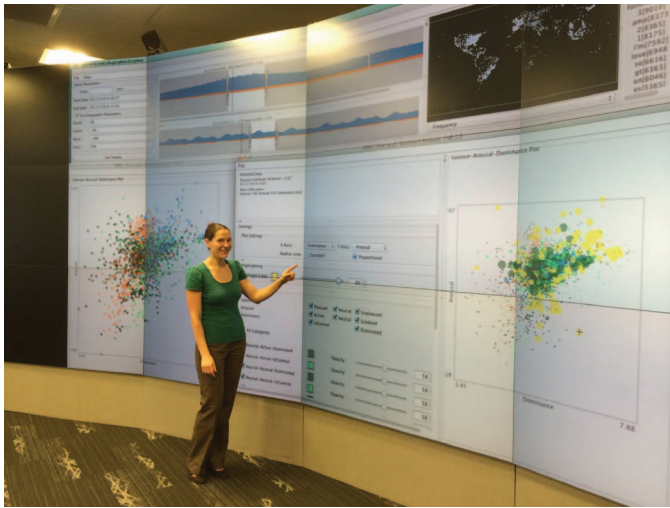


Fig. 6. EVEREST facility for analysis and visualization. EVEREST features a 37 mega-pixel display wall that accommodates stereoscopic views and can track a user throughout the room.

techniques to encode additional information about data into 3D virtual environments beyond explicit representations of the data's spatial properties. Bowman et al. describe potential applications and early research strategies in the area of IRVEs [23], and Polys et al. delve deeper into the depth and gestalt cues that affect analysis tasks within these environments [24]. User studies on IRVEs and other human-centered strategies for exploration and analysis in virtual environments will help guide the features that are prioritized in immersive visualizations for scientific analysis.

3) *Computational Challenges (Big Data)*: In general, the volume and complexity of scientific data sets continues to increase at an unprecedented rate, which fuels the current attention to big data analysis. As computational power increases and the associated costs decrease, data sets produced in scientific experiments and simulations also increase in complexity and volume. Given the importance of latency in VR experiences, we must harness the increasing power of computational machinery for big data analytics that reduce latency, particularly with the largest data sets. With point clouds and volume visualizations, we can leverage decades of computer graphics research to implement level-of-detail rendering with optimized indexing and aggregation schemes that throttle the number of graphical primitives rendered based on the virtual proximity of user's viewpoint [25]. There have been several rendering optimization schemes proposed for computer games, simulations, and scientific visualization.

In addition, we believe there is the potential to leverage distributed rendering and analytical processing so that the display system is not burdened with the full rendering workflow. For example, we have explored ways to remotely render extreme scale scientific data using GPUs on the Titan supercomputer in the Oak Ridge Leadership Computing Facility (OLCF). The resulting images can then be displayed on a 37 mega-pixel display wall, called EVEREST, with stereoscopic rendering

and human gesture interaction. The EVEREST display wall is shown in Figure 6. 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) *Integrating Automated Analytics (Big Data)*: In conjunction with intuitive interactions and powerful computing technology, we can collect human feedback to feed real-time machine learning algorithms that assist the user for large data sets. 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. This 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. For large, complex data sets where manual inspection is either undesirable or impossible, 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.

In our prototype, we capture the user's gaze to select/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.

In light of big data challenges in science, this guided analysis concept has become a necessity rather than an option. By leveraging both automated analytics and human-centered analysis, the resulting system can tackle challenges neither could solve easily in isolation. We believe this approach can also be used to improve latency, as we could remove irrelevant items. We also envision such a system could maintain a knowledge repository that stores human labels, algorithmic predictions, decisions, and results. Such a knowledge repository can be built from expert users to provide guidance to novice users and improve initial investigations of new datasets based on the similarities and results of prior work.

5) *Increasing the Adoption of VR in Scientific Domains*: We noted that VR has risen and fallen in waves over the last few decades. Today, the accessibility of VR equipment such as the Oculus Rift, promises to provide a more long-lasting, transformative effect. To ensure that we do not waste this opportunity, we must consciously explore ways to increase the adoption of VR in the scientific domains. We noted earlier that intuitive interactions that are modeled after long-standing analysis practices may help reduce the time for training and adoption of these systems. Other practical considerations

include incorporation of the domain scientists into the design process, connections to real-world scientific domains with pressing big data challenges, and smart designs that leverage both human and computer strengths. Another practical consideration is the communication of results and training information for domain scientists. The disconnect between the latest visualization advances and scientific analysis techniques has long been an issue for many scientific domains.

Also, we must validate the new systems using metrics and studies that are understood in the scientific domain as well as the Human-Computer Interaction (HCI) and visualization domains. Human subject studies and newer longitudinal studies are the gold standard for validating new visualization techniques. However, in the scientific community, more quantifiable metrics such as reduced knowledge discovery timelines, use cases that identify discoveries that VR enabled, and rates of adoption among the expert users carry more weight. As most of the research in new VR technologies will be performed in the visualization and HCI communities, we assume the former evaluations will be executed. However, the community should also ensure equal treatment of more practical evaluations that may be more convincing to the scientific community. Likewise, more traditional HCI study results should be published in scientific venues in an accessible manner to educate future users.

## VI. CONCLUSION AND FUTURE WORK

In the future, we plan to move our Unity-based prototype to a more scalable solution with hardware acceleration that renders directly to the Oculus Rift display. We have already implemented a system that renders to the ORNL EVEREST display using the full 37 million pixel resolution. An alternative solution is to integrate Oculus support into a high performance visualization system such as ParaView or VISIT. In either scenario, our goal is to develop a more generalized system that supports alternative immersive displays and incorporates hand-tracking to offer more natural interactions. We also plan to investigate the inclusion of methods drawn from the information visualization community, such as details-on-demand, context maps, provenance tracking, and user annotations in immersive systems.

Another promising area for future study is a collaborative VR system that allows users at different locations to interact and explore scientific data. Collaborative visualization with VR displays is particularly desirable at one-of-kind user facilities such as the ORNL SNS. If distributed collaborative analysis were possible, faculty at the home institution for a given research project could collaborate remotely with peers and students at the user facility as the experiment is running, which would increase efficiency and reduce knowledge discovery timelines. Finally, we believe additional research is needed to develop practical workflows in collaboration with both software engineers and computational scientists to increase the adoption within the scientific community.

Immersive virtual reality environments hold tremendous promise for scientific visualization applications. We are en-

couraged by the performance we have obtained with our prototype system, and the feedback we have received from domain scientists is overwhelmingly positive. We anticipate that continued development of intuitive interaction features will further broaden the field of scientists who can gain insight and share knowledge using VR tools.

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