

Dynamic Color Mapping with a Multi-Scale Histogram: A Design Study with Physical Scientists

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Abstract

Many research and development activities for scientific data analysis have focused on scalability challenges and data-driven features. Conversely, data visualization that focuses on models requiring human interaction rarely involve practical and large-scale scientific data analysis. Therefore, a gap exists between interactive data visualization and scientific data analysis applications. In this paper, we present a design study of interactive data visualization to support scientists who visually analyze data from neutron scattering experiments. This study was conducted in multiple phases: 1) problem characterization; 2) initial design and formative evaluation; and 3) iterative design. We characterize the problems and the design requirements for the analysis of the specific physical science data. We discuss the design, development, evaluation of our visual analytics tool and as well as our iterative developments with physical scientists. We show how to bridge the gap between the two disciplines uncovering new potential to solve their challenges in this design study. We focus on a specific challenge, finding an optimal color mapping, which plays a critical role in neutron scattering science and is broadly applicable to other scientific domains. To address the challenge, we propose two interactive visualization techniques: a dynamic color scale bar (DCSB) and a multi-scale histogram (MSH).

Introduction

Technological advances in both sensors and high performance computing drive escalations in the volume and complexity of scientific data acquired through scientific experimentation. The data acquired by such systems have tremendous potential to solve many critical scientific challenges. Also, advances in interactive data visualization techniques that integrate human sensemaking with the computational power of modern computers fosters discovery of new insight, which enables breakthroughs. However, research and development activities for scientific data analysis systems have disproportionately focused on scalability challenges while rarely considering “human-in-the-loop” approaches. The visual analytics and information visualization fields focus on human interaction techniques, but applications usually target moderate scale and tailored data sets. Therefore, a gap exists between interactive data visualization and scientific data analysis applications. By bridging this gap, we can achieve more comprehensive and timely understandings of data in challenging scientific sce-

narios – the central promise of interactive data visualization.

In particular, limited human interaction capabilities hinders the ability of scientists at the Oak Ridge National Laboratory (ORNL) Spallation Neutron Source (SNS) to understand data from neutron scattering experiments conducted at this unique facility. Physical and material scientists conduct experiments at SNS producing vast amounts of data that they analyze using a variety of scientific data analysis systems. For example, physical and material scientists often analyze data using tools that have powerful analytic features but lack task-centered capabilities. To achieve successful scientific data visualization design, task-centered design is required that explicitly incorporates user workflows and tasks into domain requirements [21].

In this paper, we present a design study on the use of interactive visual analysis to support SNS scientists who analyze data from neutron scattering experiments. Our approach for presenting this research follows the design study methodology [26, 35]. In addition to design lessons learned and insights gleaned for visualization research, we propose two interactive visualization techniques that are designed to alleviate limitations of the existing tools. This study was conducted in multiple phases: 1) problem characterization; 2) initial design and formative evaluation; and 3) iterative design. In the problem characterization phase, we met with the physical scientists to gain a better understanding of their data, challenges, and needs. We then worked together to identify a set of design requirements through iterative discussions. We then designed a prototype version of our initial framework based the design requirements and conducted a formative evaluation to evoke more feedback on our initial design. Based on the evaluation results, we iteratively refined and improved our framework. One of the interesting phenomena was that as this study progressed, they suggested new unforeseen ideas and features. While we identified several tasks in their workflow that can be addressed through interactive visual analytics, this paper focuses on finding an optimal color mapping which is one of the most critical aspects of their analysis.

To address the color mapping issue, we propose two interactive visualization techniques: a dynamic color scale bar (DCSB) and a multi-scale histogram (MSH). DCSB allows users to directly manipulate the current color mapping with simple user interactions for finding an optimal color mapping. MSH supports multiple scales in a histogram rather than one uniform scale where users can apply a small scale (fine resolution) to a specific distribution range they want to focus upon while maintaining context and the overall shape of data distribution without space distortion, and panning and zooming. These techniques can work either separately or together. In addition to the neutron scattering data, we conducted case studies on other types of data. We show how our

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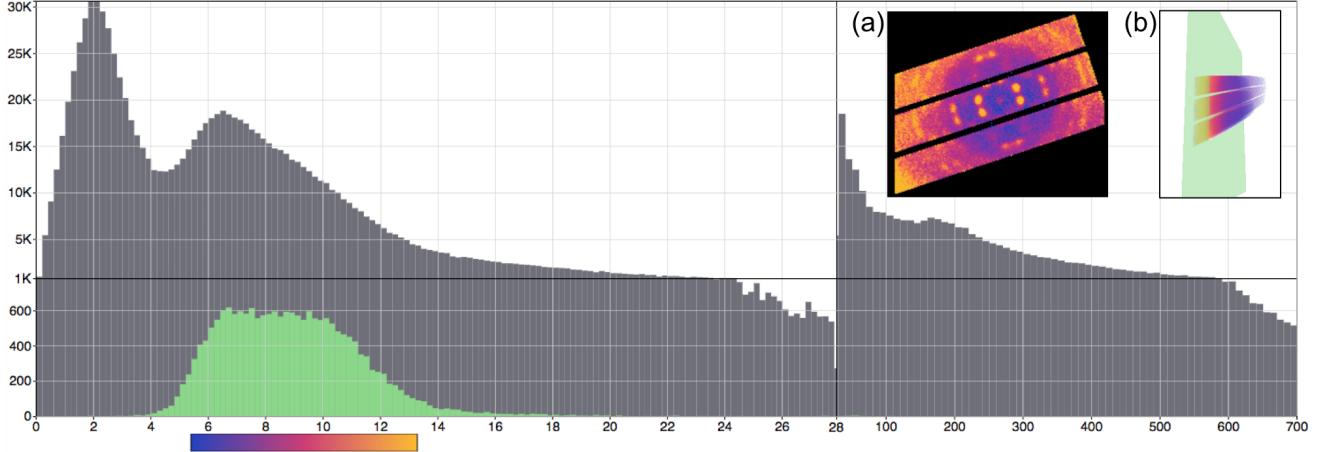


Figure 1. Dynamic Color Mapping with a Multi-Scale Histogram. The multi-scale histogram clearly represents the value distribution of not only entire data (gray), 3D volume data (b) but also the focused sub-set (green), an extracted slice data from the 3D volume. The slice image (a) is colored according to the dynamic color scale bar under the histogram.

techniques are applied to other scenarios through the case studies.

The main contributions of this paper are the following:

- We characterize the problems and the design requirements for the visual analysis of the specific physical science data.
- We design, develop, and evaluate our visual analytics tool through collaboration with many physical scientists.
- We propose new interactive visualization techniques to address a major challenge: finding optimal color mapping.
- We show how to bridge the gap between the interactive data visualization and scientific data analysis uncovering new potential to solve their challenges.

Related Work

In this section, we begin by reviewing previous studies regarding “human-in-the-loop” research for scientific data analysis. We then discuss color considerations in data visualization for two sub-topics: color scale and color mapping. We conclude the section with a review of existing work regarding multi-scale data visualization.

Human-in-the-loop in Scientific Data Analysis

Scientific data analysis has predominately focused on algorithmic speed and scalability. Scientific visualization techniques also commonly describe new visual representations, but large scale scientific data analysis research is typically not focused on “human-in-the-loop” data analysis strategies that hinge upon human interaction techniques. The opposite situation is found in information visualization and visual analytics research, where scalability and performance are usually not the main objective. Thus, scientific data analysis is ripe for disruption from the standpoint of interactive visual analysis. Nevertheless, there are some encouraging examples of interactive visual analysis for scientific data. For example, Mohammed et al. have introduced a new technique for understanding brain functions using a new interactive component that displays a 2D abstraction space [23]. Users interact with points in this space to transition between different abstraction levels of astrocytes and neurons in an flexible manner. Wang et al. have described an interactive nested parallel coordinates plot tech-

nique for explore multi-resolution climate ensembles [39]. This technique incorporates novel visual representations with a separate interaction interface for drilling down into connected geo-spatial views. The authors describe case studies involving domain experts where the experts’ feedback is analyzed to demonstrate the advantages of the approach. Our technique focuses more on direct, embedded interactions, but we also rely upon domain expert feedback as a means for evaluating and evolving the design. The concept of embedded interactions follows recent work by Endert et al. in which they argued for a “human-is-the-loop” philosophy for visual analytics [11]. Here the focus shifts to examining the user’s work process and fitting analytics into existing interactive procedures often involving direct interaction with the visual representations. Our design supports this idea of joint reasoning between machines and humans through interactive visual representations. Saket et al. have studied how user interactions influence the ability to control and decode graphical encodings [30]. Our technique uses such embedded encodings and incorporates suggestions provided in the work, such as the availability of additional feedback for the color scale and histogram scaling methods and careful design in the interaction techniques.

Colors in Data Visualization

Color is often utilized for visually displaying metric information, patterns, extrema, and other features. A *color map* or a *color scale* is defined as an array of colors that is used to map data values to the colors that are assigned to visual features in a data visualization (e.g., a graphical objects fill color or pixel values). Both terms are used interchangeably in the scientific literature. In this paper, we use the term *color scale*. We define a *color mapping* as a procedure that maps data to the colors of a chosen color scale, which involves finding optimal alignment between color and data values. The process of the using colors for visualizing data can be split into two steps: color scale selection and a color mapping. Choosing a color scale is usually done prior to the color mapping. Both steps significantly influence perception, data interpretation, and decision making [2, 29]. The methods used in the two steps, however, focus on different aspects of the use of colors. We will

now discuss these differences.

Color Scale: Traditionally, many studies have focused on color scales and many related topics [2, 29, 28, 40]. Ware [40] conducts many experiments for evaluating and comparing a wide range of color scales. Some techniques are proposed for selecting color scales, which are driven by characteristics of data and human perception to assist users to choose appropriate color scales [2, 29]. Rheingans emphasizes tasks and audiences with respect to choosing a color scale [28]. Zhou and Hansen provide a comprehensive review of color scale choices and a taxonomy for choosing the appropriate color scales [42]. Recently, Bujack et al. propose a framework to assess color scales based on a mathematical metric that mimics human perception [4]. These works mainly focus on how to design color scales regarding a color choice based on color models, such as RGB, HLS, HSV and color ordering and transition.

Color Mapping: The methods for a color mapping focus on methods to map data values to colors instead of choosing a particular pre-defined color scale. Despite the importance of this area, relatively little research has been done in this area. Colorbrewer [3] provides handcrafted discrete color pallets for various tasks. PRAVDAColor [2] and ColorCAT [22] propose tools guided by principals of the human perception to suggest a set of color scales based on data type, spatial frequency characteristics, and tasks. Although the tools allow users to choose and edit color scales, they do not focus on how to map the colors to data values. Samsel et al. propose a tool called ColorMoves [31, 33, 32] that allows users to place, move, and resize a color scale and embed it into each other on a histogram of data via an intuitive drag-and-drop process. This enables the users to interactively create a tailored color mapping for specific data and visualization goal. ParaView [1] also provides a similar function for editing a color mapping based on data. While the function allows users to handle various properties of a color scale and define a color mapping by adjusting a color transfer function, it can be difficult to use for users who lack advanced data visualization training.

Our DCSB technique also supports a similar feature, dynamic color mapping manipulation based on a histogram of data. However, we have enhanced the feature by enabling a discrete color scale and multi-scale navigation of the histogram. In this paper, we describe the improved features and emphasize the design lessons learned by collaborating with physical scientists as a design study.

Multi-Scale and Focus + Context Visualization

Multi-scale visualization techniques mainly focus on the way of data abstraction [25, 41, 9] and transition between different scales [38, 10, 8]. The techniques allow users to explore data at different scale levels and provide effective data aggregation methods. Mélange [10] introduce the design goals of multi-focus interaction for multi-scale visualization. Stolte et al. [38] use data cube aggregation and Elmquist and Fekete [9] use hierarchical aggregation to abstract data. Woodring and Shen [41] propose a technique for temporal exploration across different temporal resolutions for salient trend detection. ZAME [8] demonstrates a technique for visualizing many scale levels of a graph powered by high rendering performance. However, these techniques mainly display overview or detail level of data at one time.

Visualization techniques: *detail + overview* and *focus + con-*

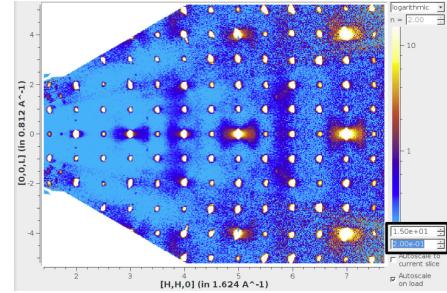


Figure 2. Using a tool (i.e., Mantid), the scientists type the min and max values corresponding to specific colors using a keyboard (bottom right black rectangle), confirm the color mapping result (left), and continue until they are satisfied with the resulting image.

text that show both overview and detail of data at the same time have many benefits for data analysis [12, 34, 16, 5]. Detail + overview displays the global overview of data and details of a selected sub-set in separate views. On the other hand, focus + context use one view for showing global context and details within the context using a visual distortion technique. Focus + context (i.e., fisheye) has advantages of displaying an area of interest in sufficient detail and spatially relating the details to the global context. A rich literature on this technique are mainly differentiated by the way of transition between the global and focus regions [19]. Vizster [15] proposes methods involving a network topology that is able to display the full detailed network of the focus nodes and the remainder of the network at increasing coarse resolutions. Stackzooming [18] provides an interactive way to show several parts of data at different levels of detail, but the separated views can hinder preservation of the user’s mental maps for the separate regions of data. Our MSH technique allows for users to magnify a distribution range of interest while preserving an awareness of the whole distribution without an additional view and visual distortion. To the best of our knowledge, this is the first work designed to support multiple scales of a histogram.

Background

The SNS at ORNL is a unique Department of Energy (DOE) user facility. Researchers from across the globe visit the SNS to execute their neutron scattering experiments for scientific research and industrial developments using the most intense pulsed neutron beams in the world. The researchers then analyze the acquired experimental data using several scientific data visualization tools. Given the expense and limited time for SNS experiments, the researchers need an effective and straightforward tool. Although the existing tools are powerful, the scientists of SNS have stated that the limitations of the scientific data visualization tools hinder the discovery of new insights which can lead to scientific breakthroughs. For example, color mapping usually requires a trial and error process in their typical approach. Nevertheless, the SNS researchers often state that uncovering significant patterns in their data mainly hinges on finding the right color mapping. This situation has motivated our investigations.

Process Overview

This design study was conducted over a period of ten months. The overall goal of this study was to support the SNS researchers in performing visual analysis of their experimental data. For this goal, we collaborated with expert physical scientists at the SNS facility. One of the scientists, who is also a co-author of this paper, leads development activities related to visual analysis of neutron scattering data and he was actively involved in planning and conducting this study. We follow the standard design study approaches [26, 35]. Our study was driven by understanding and characterizing the challenges in the visual analysis process of neutron scattering experimental data. This problem-driven design process was organized in three stages: problem characterization, initial design and formative evaluation, and iterative design.

Problem Characterization: We began by meeting with several active researchers at SNS to gain a better understanding of their needs and the details of their analytic tasks. Also, we met with senior-level researchers to get a wide and high-level of their research goals. Through iterative discussions with these domain experts we determined which challenges we should focus on and devised an appropriate action plan for solving the challenges. Our discussions involved visits to their workplaces to observe them performing data analysis tasks which helped us gain a better sense of their goals and the characteristics of their data. We then abstracted the tasks and derived design requirements for visual analysis. The characterized problems and design requirements are discussed in detail in Section, Problem Characterization.

Initial Design and Formative Evaluation: We designed and implemented a prototype based on the identified design requirements. In this phase, we also held regular meetings with the researchers to brainstorm, elicit requirements, and discuss prototypes and ideas. Our SNS collaborators also hosted a hackathon event for scientists and engineers outside of ORNL who work on neutron scattering data visualization. We presented and demonstrated our prototype at the event to gather more feedback on our initial design. The hackathon participants provided constructive feedback which translated into new needs and requirements for our work. The initial design and the formative evaluation results are reported in Section, Initial Design and Formative Evaluation.

Iterative Design: We iteratively refined and improved the prototype based on the results of the formative evaluation. In the beginning, many ideas and features were proposed, but we ruled out some features and decided to focus on the most important ones through discussions with our collaborators. The final design is discussed in Section, Iterative Design.

Problem Characterization

The goal of the problem characterization phase is to understand data, identify and abstract tasks, and formulate design requirements. Although we focus on specific aspects of the data and the tasks related to their visual analysis process, it is difficult for visualization researchers to fully understand such neutron physics data, theories behind, and specific analysis tasks. Through our regular discussions of specific concepts with the physical scientists, we gained a better understanding and applied this knowledge to the prototype designs. Also, by incorporating an expert scientist in our design team, our efforts were grounded in actual data analysis challenges and we could leverage his expertise to ensure scientific accuracy.

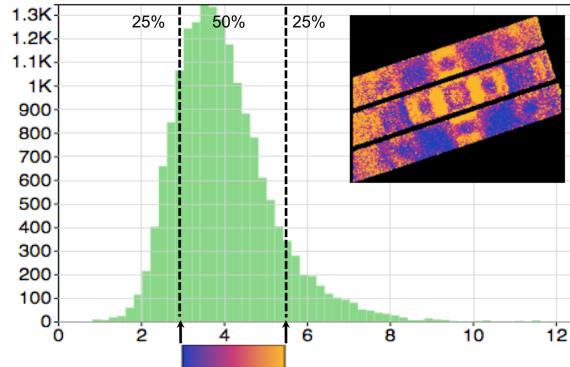


Figure 3. Histogram of a slice data of neutron scattering 3D volume and the colored slice image (upper right). The slice data are mapped by the colors vertically below of the DCSB. Color mapping is initially suggested based on the quartiles of data.

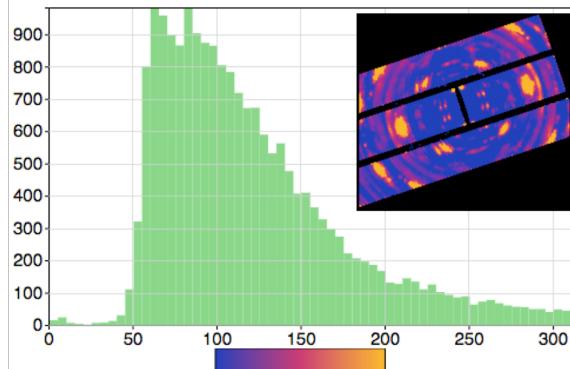


Figure 4. Histogram of the slice data of another part in the same neutron scattering 3D volume data and the slice image. The data distribution and the range of values are much different from the data in Figure 3

Data description

The SNS produces neutrons with an accelerator-based system, where neutrons are produced by a process called Spallation. Researchers from diverse disciplines, such as physics, chemistry, and materials science use SNS neutron scattering instruments to determine complex crystal structures that are described by unit cells with tens to millions of atoms. Experiments generate data sets that are large, multi-dimensional, and involve complex transformations. The size of data files produced in a single experiment may vary from hundreds of megabytes to hundreds of gigabytes, with a typical file being about ten gigabytes. Depending on the experimental configuration, billions of neutron events are measured and transformed into scientifically relevant dimensions, three of which are related to the spatial location (x , y , and z), 3D data and each location has its energy intensity value [27, 20]. SNS researchers visualize and analyze this 3D data for determining structures of their materials. Figure 1 (b) shows an example of the 3D visualization. In this paper, we focus on this visual analysis task of the data.

Task Analysis

First, SNS researchers extract a slice by specifying a 2D plane (see the green plane in Figure 1 (b)), which is intersected

with the 3D volume. Usually, the 2D energy slice is orthogonal to either the x, y, or z-axis. As shown in Figure 1 (a), the slice extraction yields a 2D array of values that are visually encoded as colored pixels in an image. The discovery of important patterns and structures in neutron scattering experiments hinges on selecting a right slice and applying an appropriate color scheme that maps the range of colors to the range of values. In both tasks, the background knowledge and intuition of the researchers are the primary drivers for finding interesting slices and patterns in a slice.

At the initial stage of this study, we focused on the first task, slice selection. We developed interactive data visualization techniques that leverage multi-touch interactions on a high-resolution display in a web-based prototype [37]. The goal of these techniques was to increase the efficiency of the volume slicing operation. After that, we realized that the second task, finding optimal color mapping is the most significant bottleneck in their analysis process. Thus, we focused our attention on the second task, finding optimal color mapping, which is the focus of this paper.

Finding Optimal Color Mapping: We monitored how the physical scientists formulate their color mappings for a given data set. After they select a specific volume slice, they then use a default color scale (often this is the rainbow color scale) to get the colored slice image. Figure 2 shows a specific color mapping tool used by the scientists. They type two values: min and max at the input fields (see the bottom-right black rectangle in Figure 2) which are mapped to the begin and end colors of a predefined color scale respectively, and investigate the color mapping result in the slice viewer at left. For this case, they are interested in specific “butterfly” patterns as shown in the slice viewer. After they get a low-fidelity sense from the initial result, they repeatedly adjust the values until they are satisfied with the results. However, if they do not have enough background knowledge of the data and experience on this process, this trial and error process becomes very time consuming and often stalls the analysis process. We were inspired here and wanted to investigate methods to enable faster color mapping design.

Design Requirements

The overall goal of finding optimal color mappings in the visual analysis of neutron scattering data is to clearly reveal important structures and patterns in the imaged data from some material. To achieve the goal, multiple requirements should be achieved. We identified four design requirements below in our problem characterization phase. After our formative evaluation, we identified new design requirements.

- **R1. Discovery:** Color mappings must support the discovery of specific hidden patterns and shapes through the visualized 2D slice image in a manner similar to the pattern shown in Figure 1 (a).
- **R2. Identification:** Color mappings must quickly assist in the identification of the values of specific patterns and shapes areas.
- **R3. Flexibility:** Color mapping should be flexible enough to support multiple scales because the experimental data sets are characterized by extremely varying value ranges.
- **R4. Effectiveness:** Color mapping should be highly effective to achieve the three requirements above. While it is nat-

ural to require effectiveness for visual analysis, the existing tools significantly lack this requirement.

Initial Design and Formative Evaluation

In the initial design phase, we prototyped an initial version of our tool based on the previously mentioned design requirements. To evaluate the prototype and evoke more feedback on it, we presented and demonstrated to many potential users during a SNS-sponsored hackathon event. We then extracted new requirements from the feedback we gained during the event.

Dynamic Color Mapping

For data analysis, color is widely used for data interpretation and visualization. A good color mapping, therefore, is essential to understanding data, discovering knowledge, and accurately communicating information. However, finding optimal matching between color and data is challenging. An optimal color mapping is also varied depending on the visualization tasks, such as emphasizing extrema, identifying clusters, and finding patterns [28]. Therefore, an effective approach is required to determine color mappings according to the objective of analysis—what they want to see in the data. Also, the definition of an appropriate way of mapping data to a color scale is complicated by the fact that there is no perfect method that produces a single “best” partition of data ranges into colors. There are recommended methods based on the statistical distribution of data, such as min/middle/max, quartiles, and quintiles, which also have certain advantages, but such pre-defined methods cannot guarantee optimal results [2]. Also, even if there are domain specific standards and conventions, there are no required rules in most cases. The reason behind our design decision is that the scientists want to arbitrarily assign colors to data according to their understanding of the data, the data characteristics, and the questions of their interest in the data (R1-R3). Therefore, we designed the DBSC and MSH techniques to enable a flexible, intuitive, and effective way for finding an appropriate color mapping to fulfill the requirements (R4).

The histogram (Figure 3) shows the value distribution of a slice of a 3D neutron scattering data. A color scale bar is placed below of the histogram. We call the color scale bar as with the DCSB technique. Here, we use a diverging color scale (blue, red, and yellow at the start, middle, and end respectively). Diverging color scales usually have a higher perceptual resolution than sequential color scales and visually divide the scalar values into three logical regions: low, middle, and high. The high perceptual resolution and the regions provide more visual cues that help to interpret data [24]. Each data value in the histogram is mapped to the color vertically below of the DCSB. For both outer ranges of the bar, we use both edge colors (blue and yellow) respectively in this mode, but it is also possible to have only the values covered by the DCSB are colored by the color scale. The image (see upper right in Figure 3) shows the resulting colored slice image after application of the current color mapping. As we mentioned earlier, the existing tools have done color mapping using matching min and max values of the data to the color scale. However, as a result of our monitoring, starting with this method often did not help enough in finding the optimal color mapping. We have observed many cases where the efficiency of the task varies greatly depending on how the scientists start with the color mapping. Thus, we suggest an initial color mapping based on the quartiles of data to

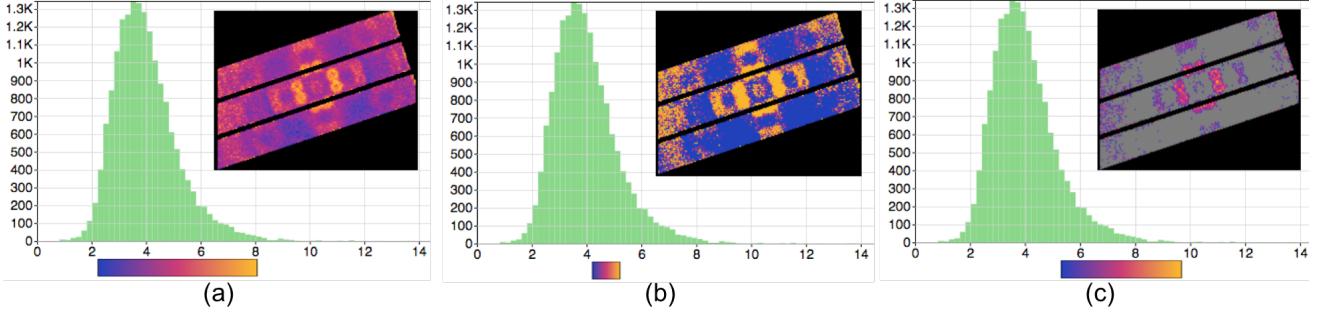


Figure 5. Users can resize and move the DCSB (a,b), and isolate a specific region of their interest (c) to find the optimal color mapping according to their analysis objectives. Each upper left rectangle displays the slice by the corresponding color mapping.

guide users to increase its efficiency. The left and right edges of the DCSB (bottom) in Figure 3 corresponds to the first and third quartiles of the data respectively. The slice image (upper right) displays the results of the initial color mapping. The scientists stated that this mapping suggestion significantly improves the efficiency of their work, especially when the user has low background knowledge of the data.

DCSB is designed to dynamically map a color scale to data using straightforward point, click, and drag interactions. Users can adjust the horizontal length of the DCSB by dragging either left or right edges and move its location by sliding it horizontally. As shown in Figure 5 (a), the extended DCSB shows more continuous patterns over the larger region than the one in Figure 3 (R1). In Figure 5 (b), shrinking and moving the DCSB discriminates the two parts corresponding to the left (blue) and right (yellow) sides of the bar. This capability can help identify the specific shapes in the slice (R1). Also, users can make specific regions visible while masking others using a single color (i.e., gray) as shown in Figure 5 (c) where only the values that are covered by the DCSB are colored by the color scale. So, users can isolate specific parts within the value range by concealing the other parts (R1 and R2).

The histogram (Figure 4) shows the distribution of another slice data in the same experimental data. The range of values is much different from the one in Figure 3. While the first and third quartiles of the histogram in Figure 3 are overall 3 and 5.5 respectively, the ones of the histogram in Figure 4 are overall 100 and 200. When they move their attention from the first slice (Figure 3) to the second slice (Figure 4), they can not reuse the first color mapping as it fits the first slice. So they need to find the new color mapping for the second slice again. By adjusting the DCSB, they can ad easily find the desired color mapping for the second slice (R4). As the user manipulates the display settings and sees the visualization change, their understanding of the data improves. At the same time, the color mapping transforms into a more suitable configuration for finding important features in the underlying data. This dynamic manipulation interacting with the data by using the control devices engages visual sense, seeing the representation change in response and then contributes to the understanding of the data and finding the optimal color mapping.

Multi-Scale Histogram

Knowing a frequency distribution of data (histogram) enables users to better understand and determine the color mapping for the data [3]. Also, the color mapping becomes a tool for in-

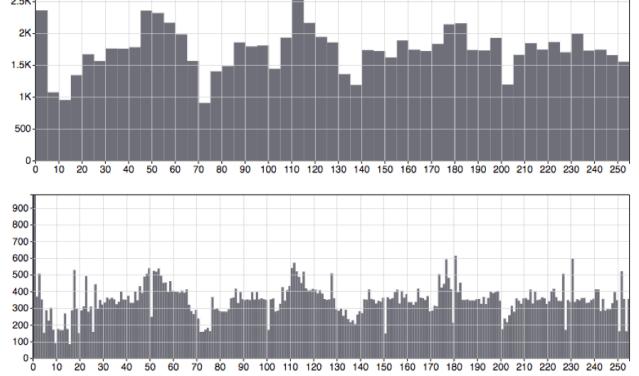


Figure 6. Histogram scale size. A large scale size shows the overall shape of the data distribution (top) while a small scale size is appropriate to represent the detail of the underlying distribution (bottom).

teractively exploring data by increasing or decreasing the value range corresponding a specific color or allocating more colors to the range for segmenting it into small parts. In fact, the scientists did not pay much attention to the histogram of the data values for the color mapping before we started this study. However, after they saw our DCSB, they gained interest in the frequency distribution information that the histogram provides. Also, they were interested not only in the histogram of one slice data but also in the histogram of the entire 3D volume data as shown in Figure 1 (b). For experimental purposes, we produced those two histograms and then superimposed them as shown in Figure 8 (a). The gray color histogram bars represents the entire data, and the green color bars are for the slice data as shown in the enlarged region (1). The histogram of the entire 3D data set is severely skewed right, which has a considerably longer tail on the right side. While the vast majority of the data is concentrated at the head of the distribution, the histogram fails to reveal the detail of the majority. Also, the difference in the (vertical and horizontal) scales of both histograms is extremely large. Figure 8 (b) shows the histograms of the same data using a smaller bin size than the previous one. Here we see that increasing (a) or decreasing (b) the bin size does not address this issue.

The basic idea behind standard histograms is that the area of each bar represents the fraction of a frequency (probability) distribution. However, a histogram is not a mathematical formula but one of the popular visualization techniques to show a data distri-

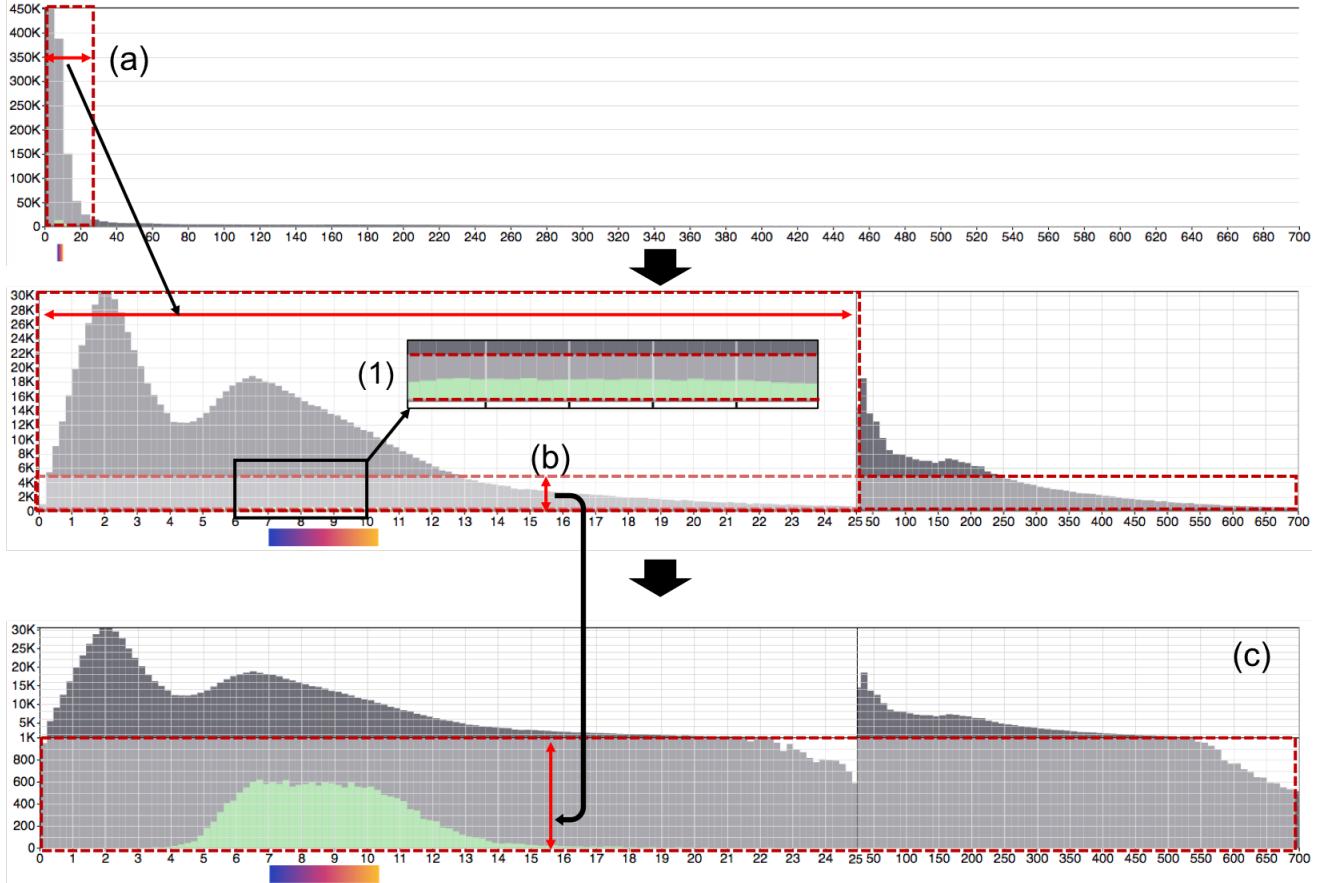


Figure 7. Visual status changes of MSH and DCSB from (a) to (c) by user interactions. Gray and green bars show the distributions of entire data and a slice data respectively. Finally, the histogram (c) shows the detail of the slice data and retains the overall context.

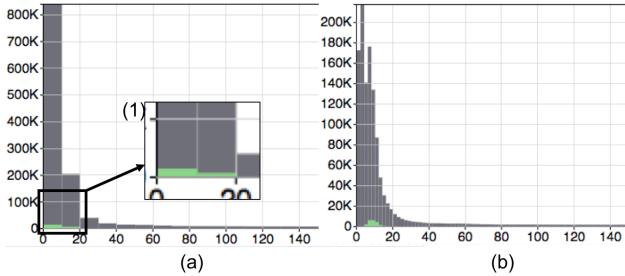


Figure 8. Using either large (a) or small (b) bin sizes of a histogram still does not guarantee good visibility of the detail of the majority.

bution. There are no definitive rules about how to bin data or how to define axes. These decisions are left entirely to the designer. Defining x -axis scale (bin size) and y -axis scale (frequency) of a histogram is a critical step for producing the histogram since the scale determines what distribution features of data shown. A standard histogram supporting only one scale for each axis has limitations in showing different distribution features of data in the same visual space. For example, Figure 6 shows two histograms which look very different but encode the same data. The scale size of the upper histogram is 2, and the bottom histogram is 0.2. Although the upper histogram is good at representing the overall shape of

the data, it fails to show the detail of the underlying distribution since the bin size is too coarse. The increased resolution of the bottom histogram shows the detail of the distribution, but the bar height at each bin suffers from large fluctuations. Containing elements that have extremely different values, some elements would be invisible when shown on one scale for a specific abstraction level. Chuah et al. [7] introduce a visualization design paradigm called selective dynamic manipulation (SDM) that seeks object-centered selection and direct object manipulation (e.g., scaling) through user control. Many interactive visualization systems inherently support this paradigm. Based on this concept, we designed a specific histogram to support multiple scales showing both an overall shape of a distribution (context) and details of a specific region of interest (focus). We keep the local focus spatially located within the global context.

The MSH technique is designed to enable multiple scales (resolutions) on both the frequency and bin size axes rather than using one uniform scale. This approach allows the user to see the detailed distribution of a range of interest while retaining awareness of the entire distribution overview. We create the histogram of both an entire 3D and a slice data and then superimposed them in Figure 7. The series of the histograms in Figure 7 illustrates the visual status changes of a histogram through a sequence of user interactions. The gray color histogram bars represents the entire

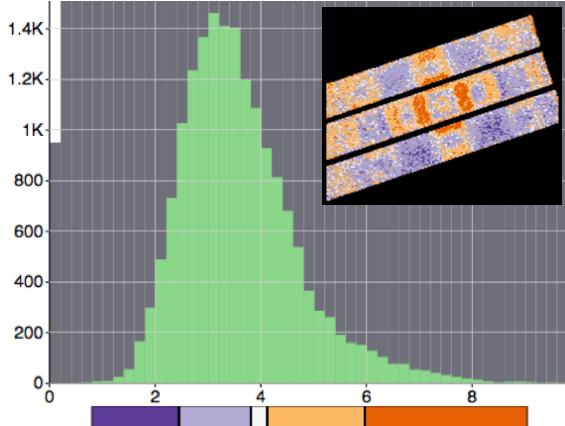


Figure 9. With the discrete DCSB technique, users can dynamically adjust the color stops (black lines) in addition to the features of the DCSB. The specific shapes in the middle of the slice image are clearly distinguished from other outer regions.

3D data, and the green color bars are for the slice data. The top histogram of the entire data is severely skewed right, which has a considerably longer tail on the right side. While the vast majority of the data is concentrated at the head of the distribution, the histogram fails to reveal the detail of the majority.

First, the user brushes the range $[0, 25]$ (a) along the x -axis in the histogram (top) and then the user horizontally extends the brush by dragging the right edge of the selected range. The extended space shows the concealed detail pattern inside the range in the histogram (middle) where the bin size of the focus range $[0, 25]$ is 0.2, and the other range $[25, 700]$ is 10. The width of DCSB component is also adapted to the extended space. Figure 7 (1) shows the zoomed region in the black rectangle in the histogram (b). However, the value distribution for the selected slice is still not clearly visible. Next, the user brushes the range $[0, 1k]$ (b) along the y -axis in the histogram (middle) and then vertically extends the brush in the same manner as above. The brushed region (bottom side) of the histogram (bottom) is scaled into the interval $[0, 1k]$ and the other region (upper side) is $[1k, 30k]$. The resulting histogram (bottom) clearly shows the value distribution of the slice and maintains the overall distributions of other ranges in Figure 7. If the newly added scale is still not enough to view the distribution, the user is able to add more scales in the same manner. Also, the user can control the DCSB component under the histogram (bottom) while looking at the slice data and the detailed majority of data. Even if the DCSB is placed between two different scales, the same way is applied. Collectively, the combination of DCSB and MSH improves the task of finding the optimal color mapping. The final representation without any highlights is shown in Figure 1.

Formative Evaluation

To gain more feedback on the initial design, we conducted a formative evaluation in conjunction with a SNS-sponsored hackathon event which included experts external to ORNL. The hackathon participants included scientists who work on neutron scattering science and engineers who develop scientific data visualization tools. The participants all had extensive practical experience with neutron scattering data visualizations. We presented the

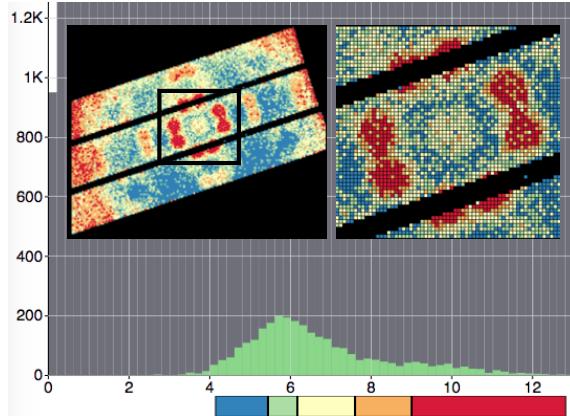


Figure 10. Users enlarge the rectangular region of interest (black rectangle) within the 2D slice image (left) and visualize it in the focus view (right). The histogram (bottom green color) represents the value distribution for the focused region instead of the one for the entire region of the slice.

underlying ideas of the design and demonstrated our prototype to these potential users during the event.

One interesting fact is that the participants have very similar problems with our collaborators. Like the SNS scientists, they stated that finding the right color mapping is time consuming but absolutely critical. For these reasons, the scientists were very interested in the techniques and gave us positive feedback on the key capabilities of the prototype. The participants recognized that they should look at histograms more for finding an optimal color mapping in their analysis process and seemed committed to adopting our approach. This situation was similar to when we first showed the DCSB technique to our SNS collaborators. Also, some of the scientists stated that the initial color mapping suggestion that uses the quartiles of data would be very helpful. They agreed that the feature would save time and assist users in finding the optimal color mapping. However, a few of them did not understand our MSH technique. It was not easy for those familiar with the traditional histograms to understand the novel feature, as is often the case when practitioners are introduced to new visual representations. Based on our experience, training through hand-on experience and incorporation of suggestions from sceptical users often alleviates such initial reactions while increasing adoption rates. Also, they stated that the MSH would not be necessary in all cases, but it would be useful if the data has elements that have vastly different values.

The feedback we gained during the hackathon event was constructive and informed us of their new needs. We extracted new requirements from the feedback. We identified three new requirements that were carried out as part of the formative evaluation:

- **r1. Classification:** Some participants stated that we should also consider the case of classifying the slice into multiple regions using specific values to clearly discriminate particular shapes from others rather than continuous patterns over a large region.
- **r2. Focus:** They often zoom in on a specific region to see the details of the region in their analysis process. However, they have to tailor the color mapping again to see the details.
- **r3. Multi-Slice:** We realized that one of the significant limi-

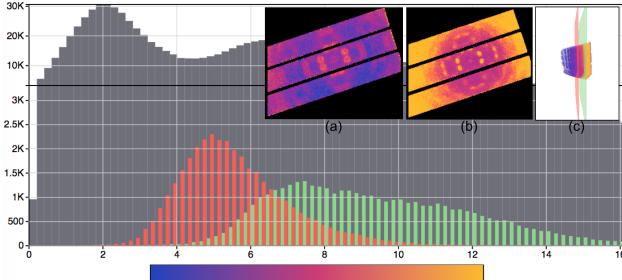


Figure 11. Multi-Slice View. Users are able to extract one more slice from the 3D volume and import it into the histogram to compare them.

tations of existing tools is that they allow only one slice view at the same time. The participants stated that the ability to compare two or more slices would be very useful.

Iterative Design

In this iterative design phase, we refined and improved the prototype based on the new requirements identified by the formative evaluation. Many ideas and features were proposed in the evaluation phase. After discussion with our SNS collaborators, we decided to add the following new features following the new requirements: discrete DCSB (r1), focus view (r2), and multi-slice view (r3). However, we excluded some features, for example, multiple DCSBs and a color histogram (coloring the bins of the histogram). ColorMoves [31] uses the similar visual metaphors as multiple DCSBs and a color histogram. Using multiple DCSBs was proposed for better classifying or providing more perceptual detail. When using multiple DCSBs, however, additional interactions arise. Multiple color scales may impose a cognitive overhead as the visual complexity increases. Therefore, we thought that for one DCSB, using a color scale with more colors or a discrete color scale rather than a continuous color scale was more useful. Using a color histogram in which the bins in the histogram are colored by the given color scale can increase the continuity between the data and the color scale. On the other hand, it has a disadvantage: some colors may appear in the slice image but the corresponding bins for those colors are too small to appear in the histogram. This situation can make data interpretation confusing.

Discrete DCSB

When we choose a color scale, we need to consider the characteristics of data (e.g., spatial frequency) and the purpose of the task (e.g., classification or identification) to increase the effectiveness of conveying information [29]. Using continuous (gradient) color scales or using more colors does not guarantee an optimal result. While controlling the color stops in a continuous color scale may be helpful, discrete color scales enable better identification, localization, and discrimination between data values [42, 36, 13]. Healey [14] proposes a systematic method for choosing effective colors where seven or less colors are optimized based on user studies.

Based on the experimental evidence and the new requirement (r1), we implemented a new feature, called discrete DCSB, that uses a discrete color scale instead of a gradient color scale. An example of the discrete DCSB is shown in Figure 9 where we

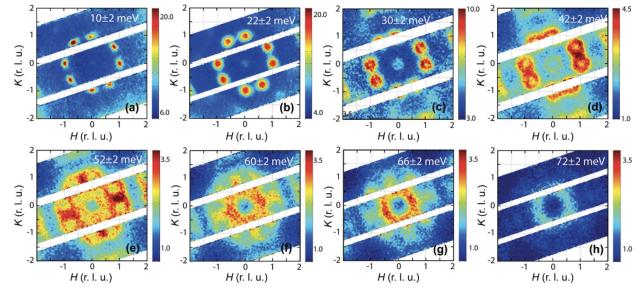


Figure 12. A series of energy slices by neutron scattering experiment [6].

use a diverging five-color scheme. Users are able to dynamically adjust the locations of color stops (black lines) in the bar and also change the size and the location of the bar in the same manner as the DCSB. We make the white color narrow and adjust other color stops and both edges of the discrete DCSB to discriminate between specific patterns (small circles at the center of the slice) and other outer regions.

Focus View

We realized that the physical scientists often enlarged a specific region and looked at the details of the region to find a specific pattern or shape. Although existing tools provide this feature, the issue is that they need to change the color mapping again to see the details in the specific region since it is fitted to the entire region. In addition to this issue, the global context disappears when zooming in on a specific region. To address these issues, we apply a technique based on *detail + overview* [17]. Users are able to select a rectangular region of interest (black rectangle) within the 2D slice image (left) as shown in Figure 10. An additional view (right) appears for displaying the details for the region of interest while the slice viewer (left) still showing the global overview (left). Then, we show the value distribution for the focused region (bottom green color bars) in the histogram instead of the one for the entire region of the slice. In addition, the DCSB is aligned with the initial suggestion based on the quartiles of the values. Then, they can also modify the suggested color mapping based on the histogram of the focused region using the DCSB. Note that the slice and focus viewers are not in the histogram in the actual system. For the DCSB, we use the discrete version to reveal the separation of the details.

Multi-Slice View

As mentioned in requirement r3, scientists conducting neutron scattering experiments are interested in investigating multiple energy slices to see the evolution of phenomena with increasing energy. For example, the sequential slices show how the small circles in the middle gradually grow, how they form a ring, and how it finally disappears in Figure 12. Their existing tools, however, do not support multiple slice views. To mitigate this issue, we improved the prototype to allow the scientist to view two slices at the same time. They are able to extract two slices (red and green) from the 3D volume in Figure 11 (c). Then, they can import the two slice datasets into the histogram where each histogram is colored in the same color as the slice to maintain the cognition continuity. The width size of the bins for the slices is the half of the ones of the global context histogram (gray), and the bins lie side by side. The red slice is visualized in the left viewer (a) and the

green one in the right viewer (b) in Figure 11. The color mapping is applied in the same manner according to the DCSB.

Case Study

In this section we demonstrate how our visual analytics design can help physical scientists in finding optimal color mapping for other neutron scattering datasets. We postulate that our techniques will reduce knowledge discovery time cycles, increase the efficiency of scientific data analysis, and have broad applications to other scientific domains. Therefore, we also discuss how our tool would applied to other data and problem contexts.

Bragg Diffraction Data: We apply our techniques into another type of neutron scattering data called Bragg Scattering. For this case, we use the discrete DCSB because the major goal of the task is to identify a specific phenomenon which is described in a specific crystal structure. The initial slice view (top right) generated by a suggested color mapping gives a user visual hints for the desired structure and then control the MSH, making the slice part (green) visible at the top row in Figure 14. The user then adjusts the DCSB to see the structure clear in the slice view (bottom right) at the bottom row in Figure 14.

Inelastic Scattering Data: Inelastic scattering data contains an additional dimension corresponding the energy gained or lost by the scattered neutron. Scientists want to discover specific curves along many directions. These curves are like a fingerprint describing the microscopic electronic and magnetic interactions inside the material. Using the DCSB and the histogram of the entire 3D volume data identifies the shape and intensity of these curves shown in the 3D volume view (top right) in Figure 15. They gain an initial insight from those and extract a slice to investigate the curves in the 2D plane. They then add one more scale into the MSH and adjust the DCSB again to see clear curve patterns (bottom right) in Figure 15.

Ozone Data: We use ozone data as an example dataset other than neutron scattering data. Each data element contains a total column ozone amount and a measuring location (latitude, longitude). The tree histograms in Figure 13 shows the distribution of same ozone amounts measured for the southern hemisphere of the Earth. The ozone amount is represented as a Dobson Unit (DU). The unit of the x-axis is DU. The color mappings are different according to the DCSBs placed underneath of each histogram. For both outer ranges of the bar, we use both edge colors (blue and red) respectively. According to the color mappings, each circle heatmap (upper right) visualize ozone amount of the southern hemisphere of the Earth. The blue color indicates where the amount of ozone is low, while the red color indicates the high area. The long DCSB (Figure 13 (a)) enables the smooth color scale that is good for showing more continuous pattern over the larger area, while the short DCSB (Figure 13 (b)) is good for isolating a specific area and showing the detail of the area (more colors used in a small area). In Figure 13 (c), we apply a discrete DCSB to the same data. The pink colors indicate where the amount of ozone is low, while the green colors indicate the high area. The average ozone levels over the entire globe is 300 DU, and the values lower than 220 DU are considered parts of a ozone hole. The values lower than 220 are indicated in dark pink, the values higher than 300 are indicated in bright and dark green. Therefore, the categorical heatmap clearly shows where the ozone hole (dark pink) is and where it is in the normal range.

Discussion

One of the most interesting facts we found in this study is that interactive visualization can involve in many domains dealing with data in any form and plays an important role in problem-solving in the domains. The important thing that we need to well understand the task and data of that domain and also to ensure that the domain people understand the underlying ideas and analysis pipeline of visual analytics. In this process, we should present as many design choices as possible and discuss them. We propose a method is that propose some existing visualization techniques that are likely to be suitable for solving their problems, discuss the techniques with them, select some techniques before starting with designing a completely new visualization method. Then, start new designs based on the selected existing techniques to be optimized for the problem. This is because they usually do not have enough experience and knowledge about visualization. We realized that they have some issues that can be addressed through existing visualization techniques, without specially customized ones. They, however, had insufficient information of what kind of visualizations are available and appropriate for their problems.

The initial color mapping feature may cause a cognitive bias called the anchoring effect, where users are anchored to the initial view they begin with. When making decision, humans tend to be heavily influenced by the first piece of information (the anchor) they have seen. For example, the initial view offered for a color mapping sets the standard for the rest of the mappings, so that views better than the initial view seem optimal even if there are other better views. As a future work, we will be looking for ways to reduce such anchoring effect, for example through visualization designs or statistical methods.

We found two limitations of the MSH. First, the multiple scales of MSH can cause misinterpretation of data when comparing the bins belong to different scales. For example, the frequency does not increase at the value 25 in the histogram (b) as the value increases in Figure 7. Since the unit size of bins at the right side of the value 25 is larger than the left side, the frequency is increased. We will investigate the ways to reduce the misreading problem. Also, if the user adds more scales into the MSH, the visual and scale complexity increases, making it difficult to interpret the histogram correctly. Therefore, we will improve the MSH to enable adjusting the existing scale to the desired focus and global context regions.

Since the scientific tools the SNS scientists currently use have a strong computation power and a wide range of features, they cannot be replaced with our proposed tool. Even, this is not the goal of this study. However, we should consider finding a better solution by using those two different tools together. We and the scientists brainstormed how to integrate our proposed techniques with the existing tools. One of the candidate ideas was exporting the color mapping and then importing it into the tools they use to support optimal color mapping design.

Conclusion

We have presented a design sturdy on applying interactive and task-centered visual analytics to finding an optimal color mapping in neutron scattering data analysis. Through iterative discussions with domain experts on every phase, this study was

<https://en.wikipedia.org/wiki/Anchoring>

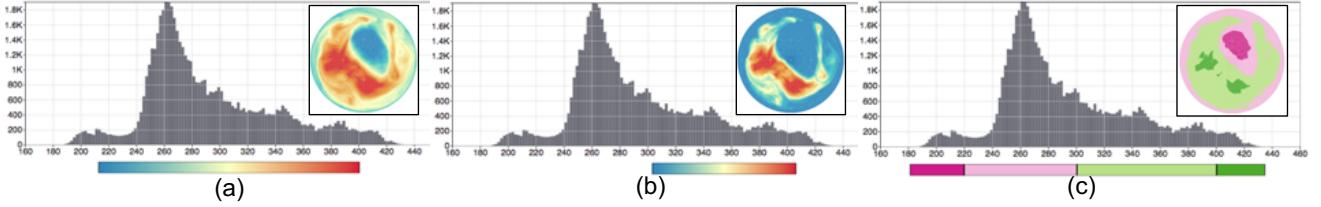


Figure 13. Visual status changes of MSH and DCSB from (a) to (c) by user interactions. Gray and green bars show the distributions of entire data and a slice data respectively. Finally, the histogram (c) shows the detail of the slice data and retains the overall context.

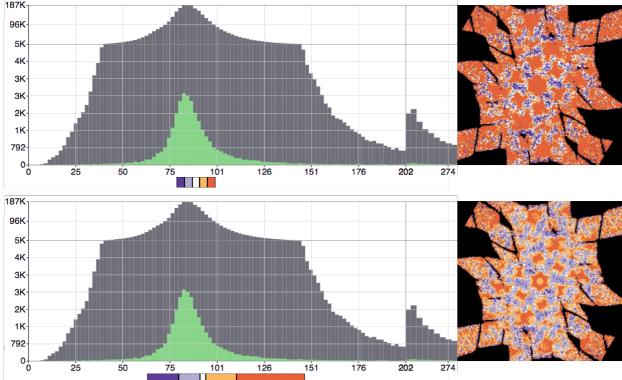


Figure 14. Bragg diffraction data. The initial slice view (top right) provides visual hints for the desired structure, and adjusting the DCSB enables the clear structure (bottom right).

conducted in multiple phases: problem characterization; initial design and formative evaluation; and iterative design. Also, we have introduced two new techniques: DCSB and MSH for improving color mapping design. DCSB provides a highly interactive and intuitive way of mapping data to a color scale. MSH enables multiple scales on a histogram for effective data distribution exploration. The combination of DCSB and MSH improves the task of finding an optimal color mapping. Our visual analytics tool was successful in improving neutron scattering data analysis carried out by the domain experts.

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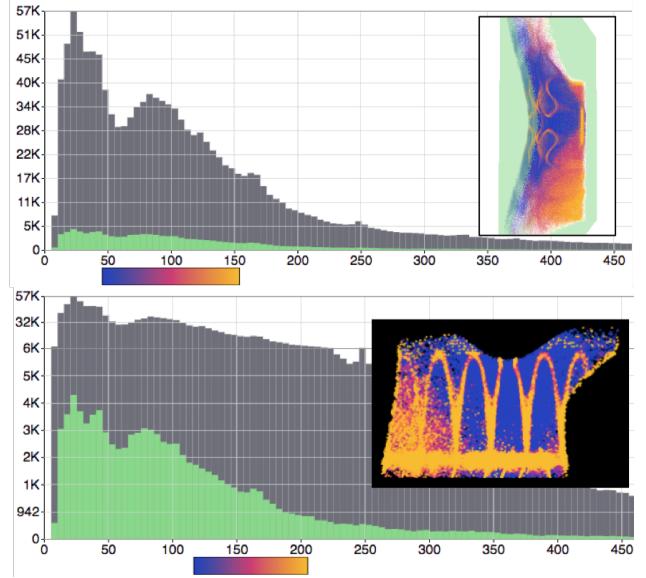


Figure 15. Inelastic scattering data. Users identify the shape and intensity of specific curves in the 3D volume view (top right) and then add one more scale into the MSH, making the slice part (green) visible and adjust the DCSB to see clear curve patterns (bottom right).

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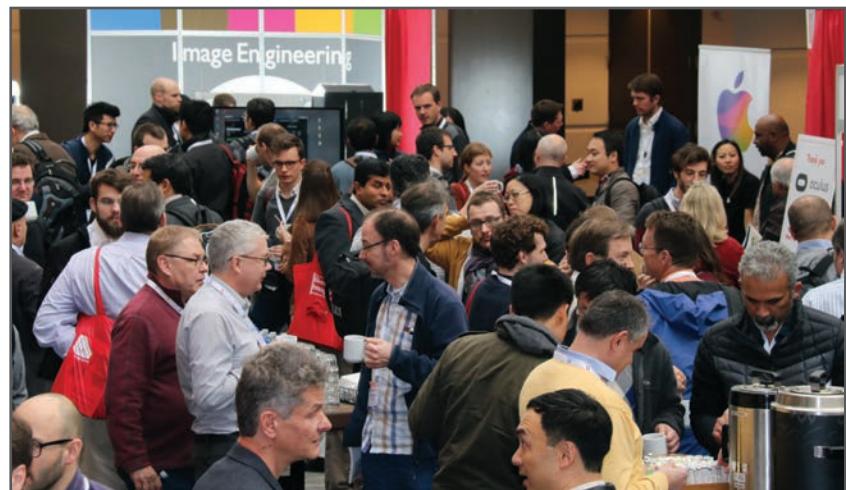
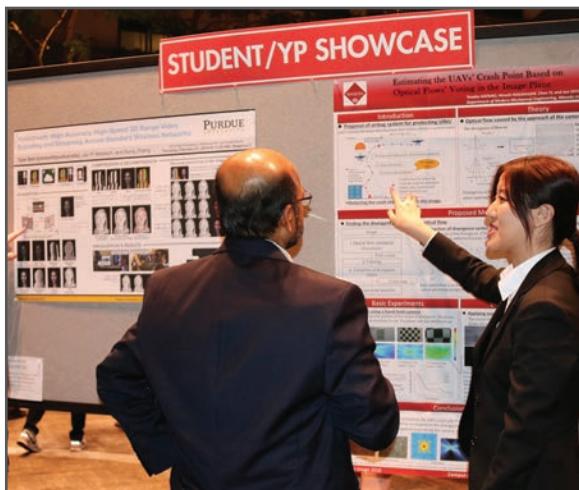
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