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Interdisciplinary Scientific Visualization

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Mouse Spinal Cord Development Visualization in Virtual Reality

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ABSTRACT

Currently, there is potential to use virtual reality visualization techniques in new applications. This semester, we demonstrated that visualizing a full mouse embryo in captured through a light sheet microscope in large scale virtual reality would benefit neuroscience researchers. Currently, the state of the art uses high end software called Bitplane Imaris [1] where scientists create videos which they use to display their data. This software only works on a two-dimensional screen. In this work established a pipeline to allow for this visualization in virtual reality. We then presented our findings to some domain experts and received feedback that demonstrated that VR could be helpful in visualizing scientific data.

Keywords: Virtual reality, human-computer interaction, evaluation.

1 INTRODUCTION

Currently there are many different applications of Virtual Reality, (VR), many of which are in visualizing scientific data. In talking to some domain experts in neuroscience, it is clear that virtual reality could be used and leveraged to help these experts to better understand their microscope data. For example, Transient Axonal Glycoprotein type-1, (TAG-1) [3] is a gene that greatly impacts the development of axons and the nervous system. There has been some work in this area and investigating how the different gene impacts the development of mice. There are still some open questions in this area. Currently, researchers are taking large scale microscope images of developing mice embryos with and without this gene. They are able to visualize the difference in the data. 3d models are currently being used on a 2d screen to investigate and visualize the data. Overall, this approach does not give the researchers a complete idea about what is going on with the data. The light sheet microscope is able to capture data on such a small scale, there is a potential to investigate this detail in virtual reality so that scientists are able to better understand this data in a more complete way. In this project we have the two following contributions. In this paper and project, we demonstrate that to visualizing this data in large scale virtual reality will help our collaborators. Second, we propose a pipeline to have this process work. We ran a demonstration with a domain expert and confirmed our prediction that virtual reality is a new and emerging technique that should be leveraged for this application.

2 RELATED WORK

VR techniques have spanned several different applications and disciplines including medical imaging [5], evolutionary biology, and many more. We are planning to take these different approaches and apply them to neuroscience data. In looking into how virtual reality has been applied to neuroscience, the applications have been focused more at looking at how they can use virtual reality to create a world for an experimental environment instead of using it as a tool to visualize their data [2] [4] Although these applications investigate how virtual reality can benefit neuroscience researchers. Much of the neuroscience data is complex and is extremely stimulating and could benefit from large scale immersive environment thus we see this a way to improve the analysis pipeline. Recently, there have also been innovations in the microscope industry such that scientists are able to capture full embryos creating data sets with small granularity but they are not using any virtual reality tools to look at this data.

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3 PROPOSED PIPELINE AND APPROACH

We propose and used three different steps in our pipeline to visualize data in the YURT. The data from a single series of measurements, yielded a result of upward of 30gb of data. The YURT is not able to handle data of this volume thus there needs to be some different ways to cut down the data. In order to have the data displayed in a useful way, our application required that we decrease the sample size while still maintaining the usefullness of the data. Through our three step pipeline, we were able to cut the data down by a factor of 100. The pipeline included 3 steps, decreasing data size using fiji, surface extraction using ParaView, and displaying the results in ParaView with the vr plugin. Currently, neuroscientists are using Imaris Bitplane to investigate their data. They are able to create videos and explore on a normal computer screen. The approach we are proposing has a similar functionality to Bitplane but is open source and allows for a more realistic comparison. This approach allows us to process the data and explore what would actually be possible given this data. The resulting approach allowed us run this pipeline on a computer with 16gb of ram.

The following sections talk about the different steps of the pipeline and some of our design decisions.

3.1 Subsampling

In looking at the data set, it is clear that having the full image set in the resulting visualization would be useful. It was clear after a period of time that this was not feasible because too much data was lost during the process of down sampling. Through this observation, it was clear that this approach would not provide the usefulness our collaborator needed.

3.2 Subsection

Instead of downsampling, the best approach was to chop the data into sub regions and find a region of interest. This approach allows the user to utilize the high granularity of the data. In our example, we cut a sub region of the rib cage. The three dimensional rendering of this image can be see in figure 1.

Since the data is still to large for visualization at this point too, there still needs to be some work in finding ways to cut down the data to have it be useful. We propose doing this through creating isocountours from the volume data. Isocountours select all the different parts of the image that have a certain intensity value and then creates a mask of that image. It then fits a sequence of triangles to this data and the resulting approach significantly decreased data size of the subsection. This process allowed us to cut the data from 3-4gb to 800mb; a data size that paraview was able to handle. There are clearly some drawbacks to this approach. Finding the correct threshold can be difficult and can drastically change how

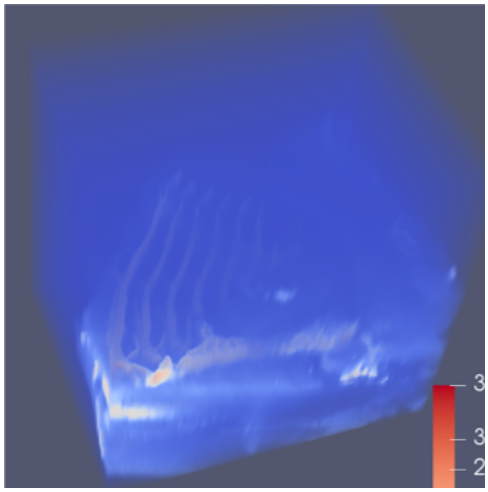

Figure 1: 3D Volume data from subsection displayed in ParaView

the surface appears. Overall, in this work we used a simple search technique using the transfer function on Paraview. This allows the user to see what data is important in the visualization and can give a good estimation of what would make an interesting surface to look at. There are other process that will work for this approaches will allow for more useful isosurfaces. The following are two isopotentials derived from the above approach.

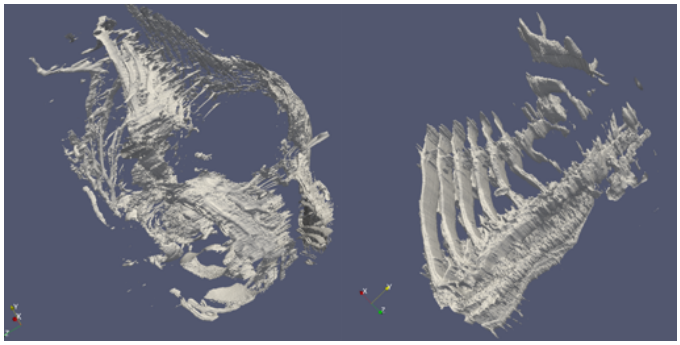

Figure 2: Surface Rendering from Volume data in ParaView

3.3 YURT Visualization

The last part of the pipeline was running ParaView with the VR plugin on the YURT. ParaView works to read and view the data. The VR plugin then adjusts the view to work with a VR display. There are some more components that need to be fixed though to have the full pipeline to work. For example, head tracking did not work so the collaborator could not zoom in and interact with the data. Below is a picture that shows the view in action.

4 Experiments

To verify our hypothesis, we had 2 experts come in and check out the virtual environment. They are experts on the state of the art and we asked them a sequence of questions about how they like the visualization. The resulting section talks about the experimental setup and the experimental results.

4.0.1 Experiments Setup

The following sections are summarizations of the responses to the questions asked during the demonstration. How does this tool compare to the tools you use? This tool provides some value that their current tools cannot do. For example, originally, they looked at single microscope images to interpret data. Now they use a sequence of images on a display. Through this visualization, they can get some usefulness and it is clear that they could get an improvement in looking at this in VR

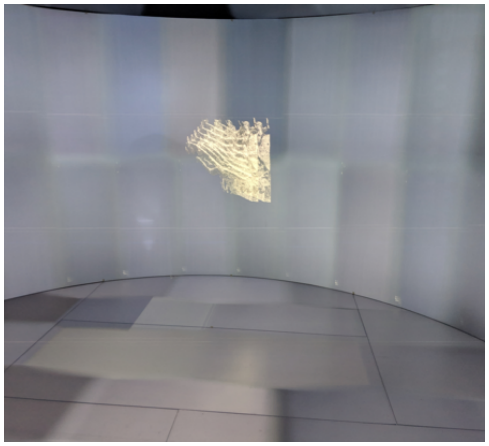

Figure 3: Image of Visualization in the Yurt

4.0.2 Do you expect to get some value out of a tool like this?

Yes, it is clear, even with the surface rendering they could see different features that they could not see on the screen earlier.

4.0.3 What are the features you would like to see in a tool like this?

They saw that they would like to be able to create different isopotentials and change the different thresholds and display them as they are created.

Overall, we see that there needs to be a larger scale user study to verify the results. It is clear that process would allow for more conclusive results.

5 Conclusion

Overall, it is clear that there is some benefit for the virtual reality environment. That being said there needs to be much work to have it replace that of the state-of-the-art techniques and it is clear that those tools may not be completely replaced. It is clear that visualization in virtual reality is helpful and would be a cool tool to use to explore this dataset more completely. There needs to be some work though in make the pipeline clearer and easier to document. In looking at this work there are several open questions. One is what are the different features that would be valuable to scientists for the visualization for a virtual reality tool? For example, should there be ways to create different animations or finding ways to manipulate the data? These questions will continue to look at if virtual reality make sense as a tool to use in visualizing and exploring data.

It is clear though that virtual reality is another tool that can be utilized to look at neurosicience data through using our pipeline, researchers can use large scale virtual reality to look and investigate their data, and thus find some usefulness.

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Visualization for Chemical Multi-Spectral Space

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Abstract

Each molecule lives in a unique position in the "chemical space", where the coordinates are determined by the properties of the molecules. In this work, we have developed an approach to explore the chemical space of a set of molecules with their multi-spectral data - NMR and IR. By generating fingerprints of the molecules from their spectral data and calculating their similarities, we are able to create, analyze and visualize an undirected graph. It is shown that similar structures lead to similar spectra, resulting in areas of nodes in the chemical multi-spectral space. Sub-areas may also exist in some large areas. It will be helpful if more work can be done in the future, like improving the methods and doing evaluation.

Keywords: Chemical Space, Chemical Fingerprints, Chemical Similarity, Graph Drawing

1 Introduction

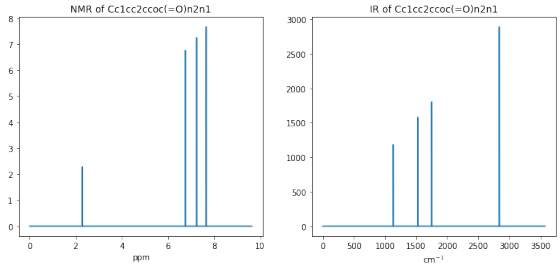

Figure 1: An example of 2D-plots for NMR and IR spectra.

There are millions of possibly useful molecules for molecular computing [1], which makes it very challenging to visualize their properties together. The "chemical space" is a concept to resolve this problem, by defining multidimensional property spaces where each point has the coordinates describing the properties of one molecule. People are using different properties to visualize the chemical space [2][5], but no one has done it with the "multi-spectral" properties such as NMR and IR spectroscopy. The conventional way to analyze one piece of spectral data is to display it in a 2-dimensional plot (spectrum, as shown in Figure 1). Therefore, in this work, we has developed an approach to explore the chemical space from multi-spectral data.

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2 Methods

2.1 The Dataset

We have included a subset of molecules from the GDB-13 database of small molecules[4] in our dataset. The subset is the molecules that have a common molecular weight 150. There are in total 1297 molecules in this dataset. We have done computations on these molecules to get the theoretical NMR and IR data. A NMR spectrum is represented by dividing the continuous data into 9635 bins, whose widths are all 0.001 ppm. An IR vector has 53363, 0.067 cm^{-1} bins. See Figure 1 for example.

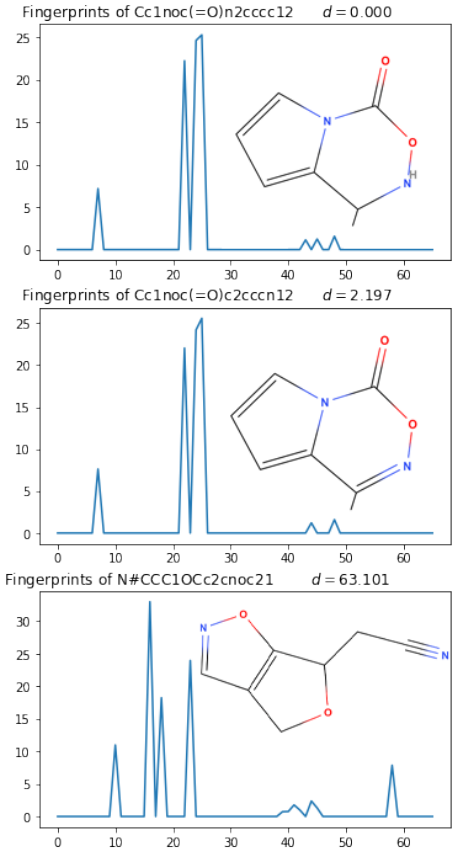


Figure 2: Examples of fingerprints and similarity values

2.2 Chemical Multi-spectral Fingerprints

Fingerprints are generated by combining nearby bins into a new one, and concatenating NMR and IR. The widths of new bins are chosen to be 0.3 and 111.7, for NMR and IR, respectively. A constant 0.1 is used to scale the values of IR, since it is not in the order of magnitude as those of NMR.

2.3 Similarities

Euclidean distance $d(\vec{f}_1, \vec{f}_2)$, which is just the length of the difference between two vectors of fingerprints, is applied to calculate the similarities between the fingerprints.

2.4 Graph Making

The Euclidean distance is transformed to similarity value by the following equation: $w(e_{1,2}) = 1 - \frac{d(\vec{f}_1,\vec{f}_2)}{\max_{e_{i,j}\in E}\{d(\vec{f}_i,\vec{f}_j)\}}$. Every molecule (fingerprints) is treated as a node in an undirected graph, where edges are constructed by a threshold 28 of distance, and the weights are assigned by the similarity value.

2.5 Visualization for Graph

The visualization for the generated graph is achieved by the software Gephi [3] with the layout algorithm called ForceAtlas2 [6], which is a force-directed graph drawing algorithm. The force has four components: a classical attraction force, a repulsion by degree, gravity to keep the nodes in the visualized area, and a component describing how the edge weight effects the force.

3 Results and Discussion

3.1 Fingerprints and Similarities

The generated fingerprints are 65-dimensional vectors. Some fingerprints are demonstrated in Figure 2 for example. We can see that molecules with similar structures have similar fingerprints, and the Euclidean distances to the first molecule also show that.

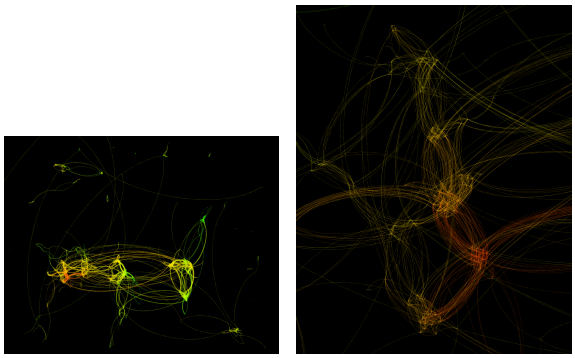
3.2 Graph Generated from Euclidean Distances

The overview of the graph which is generated with Euclidean distances is shown in Figure 3(a). All the nodes are colored according to the Euclidean distance to the base fingerprints (that of the molecule "Cc1noc(=O)n2cccc12"). Following the order red, orange, yellow, green and cyan, the similarity decreases. And the color of each edge is mixed by the colors of the two nodes it connects. We can see most of the nodes are positioned in several areas, which means the corresponding molecules can be somehow grouped by their spectral data. Also, there are points scattered in the figure, because those molecules are too different from others.

If looking into details of the graph, we can find there are also sub-areas in the areas, as shown in Figre 3(b). Moreover, The reddest group is shown in Figure 3(c). It is as expected that all the nodes here represent molecules with similar structures.

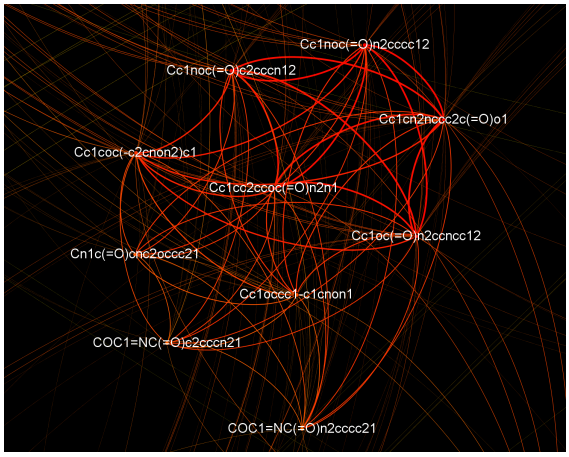
4 Conclusion

We have explored the chemical multi-spectral space for 1297 molecules by making a graph from the similarities of their spectral data. Euclidean distances seem to be more suitable



(a) Overview of the chemical space

(b) Sub-areas in the chemical space



(c) A group in the chemical space with the labels of names

Figure 3: Visualization results

than Cohen's Kappa to be used as the similarity measurement. To visualize the generated graph, we have used a force-directed drawing algorithm, and the results are pretty good. It shows that similar structures lead to similar spectra, and then result in areas of nodes in the graph. The graph drawing method indeed shows the relations among the nodes.

We have introduced a way to deal with spectral data of chemical molecules in the chemical space. It will be helpful if further research is done to improve the method, e.g., to have better parameters and a better scale factor for generating fingerprints, or to make the process more interactive where users can select any node as they like to be the base and the colors will change as the selection changes. User study will be worthwhile for evaluating this visualization method. Moreover, other dimension reduction methods may also be useful to handle the complicated data.

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Immersive VR vs Non-VR Visualization for Evaluation of Vascularization in 3D Tissue Engineered Grafts

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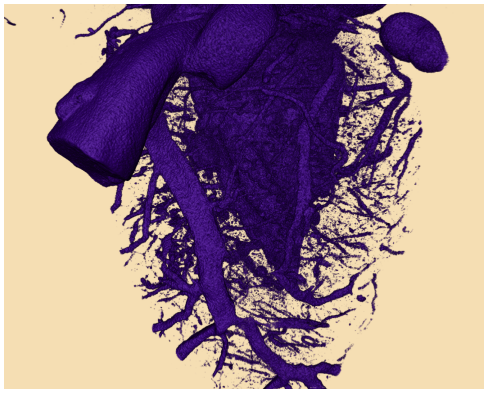

Figure 1: 3D volume rendering from opensource VTK software, showing 1/4 of blood filled areas within a rat heart

ABSTRACT

We present a case study to assess the utility of immersive virtual reality for visualizing vessel integration into tissue engineered heart constructs from micro-CT data. Vessel integration is one of the most important aspects of engineering live 3D tissues, as no blood flow means the tissues can not survive. Using a novel application of volume rendering, we visualize these vessel maps in an immersive virtual reality environment to get a greater visual understanding of how the vessels integrate in the various vascularization inducing conditions. We assessed if researchers find the VR representation of the data more conducive to deductive reasoning than the standard 2D viewing techniques by coding the transcriptions from our think aloud study and counting instances of positive and negative key phrases.

Keywords: Virtual reality, human-computer interaction, evaluation, perception, scientific visualization.

1 INTRODUCTION

Consumer-level virtual reality (VR) hardware is becoming more readily available and affordable. Head-mounted VR, such as the Oculus Rift and HTC Vive, are particularly popular due to their their low commercial price. The HMD's provide an immersive experience that allows for users to have a higher degree of interaction with a visualization. This ability to be immersed in a scientific data set allows for increased perceptual ability by researchers. The increased resolution as well as the increased depth perception within the 3D data set allows for improved visual parsing of the dataset for research interests.

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1.1 The Application

Heart Disease is the leading cause of death worldwide [1]. Developing a therapy to repair or replace damaged heart tissue rather than replace a whole heart, could be invaluable for bettering patient outcomes. Creating a therapy to replace damaged heart tissue requires engineering 3D heart tissues in vitro that reflect the nature of the native heart tissues. One of the major roadblocks to engineering tissues is inducing vascularization[1]. Vascularization, or inducing blood vessel growth into tissues, is important as blood flow is vital to the survival of the tissue. If the vessels do not distribute evenly and quickly throughout the tissue, then the tissue will die. So investigating how vascularization occurs in these heart constructs in vivo, is important for developing viable engineered heart tissue. Micro-CT imaging allows for visualizing the development of new vessel formation in animal models and elucidates to the efficacy of each bio-engineered construct in facilitating heart muscle tissue repair [2]. The whole-heart vessel maps hold information about what kind of vessels, where vessels originate from, and how they integrate into the graft. Evaluating these on a single quantifiable measure would not allow for simultaneous consideration of each of these properties. The current method of viewing the 3D vessel maps doesnt allow for full resolution of each of these various pieces of information at once, and thus an immersive method of visualization would provide a better view of how these vessels relate within the whole-heart.

The work presented in this paper makes the following contributions toward improving the methods of viewing and assessing visualizations of 3D heart constructs:

- We describe the most readable open source method for displaying/visualizing our small vessels from Micro-CT data.
- We create an annotated list of open source software for volume rendering 3D virtual environments.
- We conduct a user study an analyze results from a user study

to make determinations about the usefulness in VR for scientific inquiry on Micro-CT vessel data.

2 Related Work

Others have shown that 3D imaging of bio-engineered constructs is the preferable method of viewing tissue and vessel integration. Guldberg et al. shows how the use of 3D imaging is preferable to other methods of viewing vessel data as it provides more opportunity to comparatively understand the data [3]. Meisner et al. compares the volume rendering algorithms when viewing various data sets for their timing and quality of image production [4]. Bade et al. compares the Mesh smoothing algorithms for visualizing medical data [5]. Shelmerdine et. al, have shown that 3D visualizations of microCT data are beneficial for garnering more information from the micro-CT datasets [6].

In terms of evaluating the utility of immersive visualization for this particular vessel dataset: Laha et al. describes the benefits of immersively visualizing 3D volume rendered micro-CT data. In this paper they describe that the field of resolution or FOR was the immersive factor that had the most impact on the qualitative user outcomes [7].

3 Methods

We carried out our experiment at Brown Universitys visualization lab within the Center for Computation and Visualization. The experimental setup included a desktop computer and HTC Vive headset, controllers, and base stations. Participants were asked to interact with the dataset renderings on the desktop first, and then using the Vive.

The participants were given microCT data of a rat heart with a voxel size of 0.1 x 0.1 x 0.1 mm. We used 1301 slices with a resolution of 512 x 512 pixels to show the top left quarter of the rat vessel map. Desktop visualizations of the top left vessel map were developed using surface and volume rendering techniques on ParaView, an open-source interactive application built on top of the Visualization Toolkit (VTK). The application used for the Vive experience was OpenVR, a VR plugin integrated into ParaView.

We recruited three discrete groups of participants, with each group consisting of two individuals. The participants were grouped by type of experience - biomedical researchers, experts in scientific imaging, and students studying VR. For every study session, we brought the pair into the visualization lab and began by introducing them to the equipment and dataset. We also informed the participants of a camera placed in the room to video record the session. To begin the trial, we asked the participants to interact with the data and talk to each other about their thoughts on the visualizations. Participants were prompted to keep talking if there was a silence for longer than a minute. After the participants finished interacting with the dataset, they were each asked which visualization they preferred and for a reasoning for their selection.

To analyze the data from the think aloud study, we coded the transcriptions from the think aloud study and counted the instances of positive and negative key phrases. These phrases we categorized as clarity, understanding, interaction, future thoughts, and artifacts. These different phrases tell us different information about how the users interact with the different virtual environments.

4 Results

The counts of the instances for each category of coded words were separated by user study condition (VR or Non-VR). In terms of clarity, there were more instances of the positive and negative phrases for the Non-VR condition. While there were less instances of positive clarity in the VR condition, this could be due to researchers unfamiliarity with working with VR. We could control for this confound by introducing a training module into the user study prior to testing the study conditions. There were more positive and negative instances of interaction comments in the VR condition, and the VR condition had more positive interaction comments than the Non-VR condition. For the understanding condition, both conditions were similar baring the Non-VR condition having one more instance of a positive understanding comment.

I would say that, that would be difficult to tell. (that = disting	VR	Und	2R
But you do see more than you see on the flat screen, I thin	VR	Clar +	2R
What I like actually is the moment you stick your head insi	VR	Clar +	2R
What do you do with the controller again? Just make it sm	VR	Int -	2R
The 3d one is so much better and the uh, when you look a	VR	Clar +	2D
the stereo display is a significant advantage for trying to ur	VR	Int +	2D
yea, if you make it come closer or further away and you po	VR	Int +	2D
It would also be interesting to compare this to a shaded su	VR	Inf	2D
And that's one of the things that you can see here. If you z	VR	Clar +	2D
So I'm noticing large vessels on the periphery.	Non-VR	Clar +	1K
which is good because the main arteries and veins will be	Non-VR	Und +	1K
they look a little pixelated and broken	Non-VR	Clar -	1K
Some of that looks really nice in there.	Non-VR	Clar +	1K
Especially when you start to slide things left or right in ther	Non-VR	Int +	1F
because those look real to me.	Non-VR	Und +	1K
I would wondering if this area would do really well be trans	Non-VR	Inf	1K
So that is the major one for me as it shows it is going into t	Non-VR	Clar +	1K
If you could click on that and and show which one it conne	Non-VR	Inf	1K
But even here it seems like you could almost kind of follow	Non-VR	Int +	1K
ts a little twisty and bendy. It kind of comes up front to the f	Non-VR	Clar +	1K
See that one coming up and in and around and kind of bra	Non-VR	Clar +	1K
So the way you cut it off But this way too does help see tha	Non-VR	Clar +	1K
And If we do an arrow to the area and say here it is and pu	Non-VR	Und +	1K

Figure 2: A subsection of the coded table of phrases pulled from the think aloud user study video transcription.

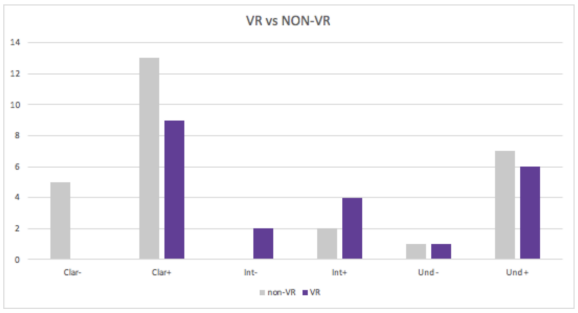

Figure 3: VR vs NON-VR Counts of Coded Words

Due to our sample size, these numbers are not necessarily representative of the usefulness of VR. Making edits to the controls of our user study as well has creating more strict procedures for analyzing the results from the study could provide more concrete results. In addition, many of our participants were not familiar with viewing this kind of data in VR which is reflected in the count of artifact coded phrases. VR had all 6 instances of ”artifacts” which are coded as any vague complement that can not be attributed to anything other than surprise or unfamiliarity.

5 Conclusion

We have created a pipeline for processing and creating a virtual environment for microCT vessel data, which can be used in the future. Due to the sample size as well as the confounds that became apparent during the conduction of the user study, any strict conclusions can not be made. The data shown is quantitatively inconclusive, and a more controlled user study method as well as improvements to the virtual environments could drastically change the results.

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