

## Example of a Research Plan

I. Virtual reality and ray tracing for computational materials science

II. Investigators:

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Computer Science, 2018

SPIN Mentor Name, Title  
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III. Hypothesis, Research Questions, or Goals of the Project

The goal of the project is to create a 360-degree video that illustrates the change in electronic density when hydrogen passes through aluminum foil. The video could be in virtual reality via Google Glass.

The research questions to be addressed are:

- 1) How to render frames with a stereo-spherical view
- 2) How to combine all rendered pictures into a virtual reality video

IV. Background and Significance

a. What did previous research reveal?

Previous research reveals that virtual reality can provide an intuitive and interactive interface for scientific visualization. (Virtual Reality in Scientific Visualization P 65)

b. What has been explored and discovered?

YT's newest version has developed virtual cameras with transfer function to render

c. What factors have influenced the outcome?

The transfer function chosen for visualizing isosurfaces, spherical camera position, camera movement as the chemical reaction progress.

References:

- 1) Tomasz Mazuryk and Michael Gervautz. Virtual Reality, History, Applications, Technology and Future, 1996. Source: <https://www.cg.tuwien.ac.at/research/publications/1996/mazuryk-1996-VRH/TR-186-2-96-06Paper.pdf>

- 2) Steve Bryson. Virtual Reality in Scientific Visualization, 1996. Source: <http://cumincad.scix.net/data/works/att/029b.content.pdf>

V. Research Method, Design and Statistical Analysis (if applicable)

The first research question will be answered by developing functions to stereoscopically render density data files.

The second research questions will be answered by exploring documentation on how to create virtual reality videos.

VI. Potential Benefits

This research will provide an example for visualizing density changes in virtual reality setting and serve as a reference for future visualizations.

## Example of a Research Report

- I. Virtual reality and ray tracing for computational materials science
- II. Abstract/Synopsis

We have created a python script to parse the original data file and render density isosurfaces with a stereo-spherical camera. With data files on a consequent timeline, we are able to create a 360 degree video on secondary electron simulation.

- III. Methodology

We used yt library to create a rendering script for the electronic density files. In our script, we preprocessed the original data, specified the transfer function of isosurfaces, and create a virtual stereo spherical camera at the location of the hydrogen. The camera is original looking perpendicular to the aluminum foil, and the users can look around the environment by dragging their mouse or finger on the picture or video.

- IV. Introduction and Literature Review

The purpose of scientific visualization is to graphically illustrate scientific data to enable scientists to understand, illustrate, and glean insight from their data. [Wikipedia, scientific visualization] In [2] and [3], it is argued that virtual reality provides a more natural and interactive environment, and therefore facilitates scientists to draw insights from 3D data. The purpose of our research is to develop virtual reality visualization for secondary electron simulation and enable the user to view the electronic density in 360 degree around the hydrogen.

- V. Results and Conclusion

We are able to generate a 360 degree stereoscopic video that follows the position of the hydrogen. A rough draft of the video can be found at <https://www.youtube.com/watch?v=g-sd2xlqNdg>. The users are able to explore the electronic density environment while following the hydrogen's movement through the aluminum foil. The virtual reality video provides the users a more immersive and comprehensive view of electronic density data.

- VI. Discussion

Our script and video serves as an example for future virtual reality visualization on similar scientific data.

- VII. References

- 1) Tomasz Mazuryk and Michael Gervautz. Virtual Reality, History, Applications, Technology and Future, 1996. Source:

<https://www.cg.tuwien.ac.at/research/publications/1996/mazuryk-1996-VRH/TR-186-2-96-06Paper.pdf>

- 2) Steve Bryson. Virtual Reality in Scientific Visualization, 1996. Source: <http://cumincad.scix.net/data/works/att/029b.content.pdf>
- 3) Michal Koutek, Computer Graphics & CAD/CAM group, Faculty of Information Technology and Systems (ITS), Delft University of Technology (TU Delft). Scientific Visualization in Virtual Reality: Interaction Techniques and Application Development, 2003. Source: <https://graphics.tudelft.nl/Publications-new/2003/KO03a/KO03a.pdf>