3D Visualization of Hydrodynamic Factors Influencing Mineral Dissolution

Joseph Berman[a], Rakshan Joshi[b]

[a] Northeastern University, Boston, MA

[b] Poolesville High School, Poolesville, MD

National Institute of Standards and Technology
U.S. Department of Commerce

Applied and Computational Mathematics Division

High Performance Computing and Visualization Group

Introduction

While conducting an experiment focused on studying the topography of a calcite mineral sample under a stream of flowing water, researchers collect abundant amounts of data. Through the process of data collection during the experiment, the researchers collect millions of data points for various attributes of the mineral, such as topography, dissolution, and concentration. Interpreting and visualizing this data is an obstacle faced when analyzing the results of the experiment. We have taken that large amount of data and represented it visually in a 3D environment in order to present a form of visualization of the data. Possessing a method of physically viewing the data offers a more hands on, viewable approach to data analysis for researchers. The CAVE (CAVE Automatic Virtual Environment) is the configuration in which the researchers view the data in three dimensions. The CAVE is a series of projectors and screens that can map a 3D model in an immersive view.

Photograph of the experimental setup

Process

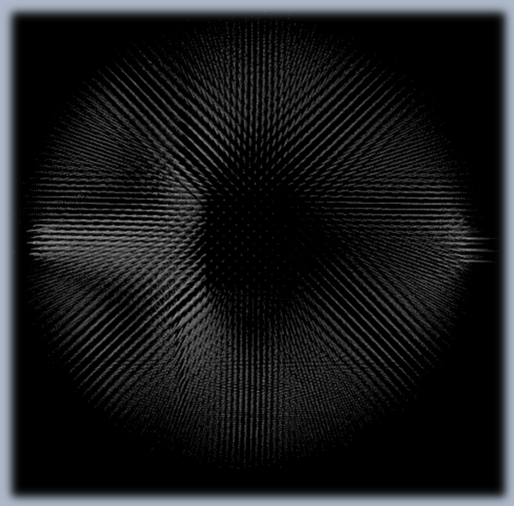
There were two different types of data received from the experiment. The first one is water flow vectors, while the second data set regarded mineral concentration. The purpose of modeling these two data sets was to view a possible correlation between them, possibly indicating to researchers a deeper understanding of the data.

Water Flow Vector Field

The researchers presented data of the x, y, and z vectors of the flow of water during the experiment. The dimensions of the environment are 155 x 155 x 39, which translates to 936,975 data points. Each data point contained these 3 vectors. From these vectors, we made one resultant vector that represents the direction and speed of the water at that point. Each resultant vector is created, rotated, and translated using HEV(High End Visualization) utilities, and was implemented through the use of python. The vectors are represented by cones, as the tip of the cone indicates the direction of water flow at that point. The end result is a field full of vectors.

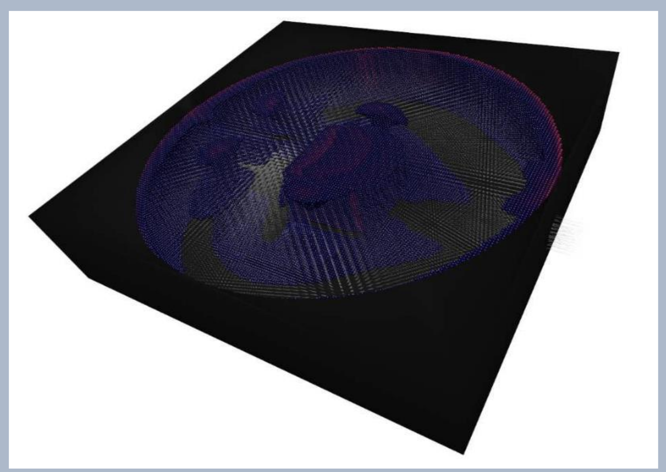
Mineral Concentration Animation

The second aspect of data modeling, mineral concentration, differed from the vectors as this was an animation rather than a still frame. This animation had 92 pages(frames) of data. Therefore, it contained 92 times more data than the vector field. The first step was to split the data into 92 different data files so that reading the data could be done faster. Next, HEV utilities were once again used to make spheres at each point that represented the concentration of the calcite. To display values of varying concentration, the color of each sphere was changed. In this case, the colors varied from blue to pink, with higher concentrations represented as more pink of a color. Once all 92 frames were modeled, they were played in succession to represent the running animation. Additionally, this animation was implemented through Java.

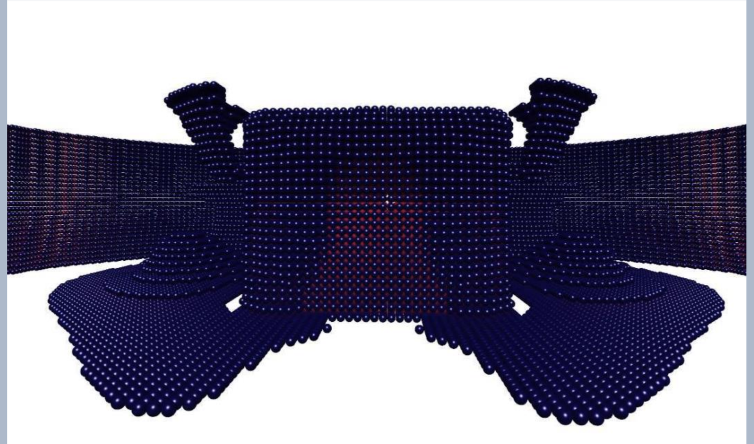


3D model of the entire vector field

Immersive view of an inside section of the vector field



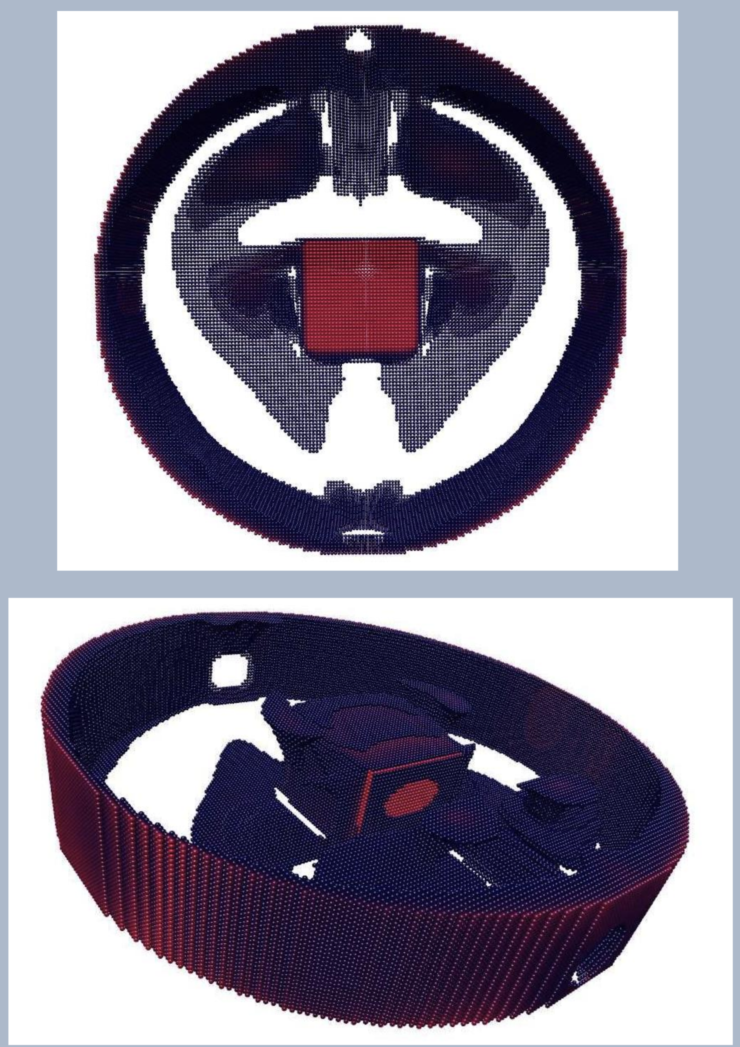
Vector field and the last frame of the concentration field combined into one display



Concentration surrounding the mineral sample during the 92nd frame

Results

Both models clearly took a circular shape, as that was the shape of the experiment's environment. Furthermore, there is a large cube-shaped gap in the vector field, along with a pink cube in the concentration field. This was clearly caused by the calcite sample itself, as no water can flow through it and the concentration is highest there. The most significant observation, however, is the presence of a correlation between the two data sets, as speed and concentration were inversely proportional. This showed us that at every point with a low velocity, there was a higher concentration, and at higher velocities, there was lower concentration.



The 3D model of the last frame of the concentration animation

Conclusion

The researchers discovered a series of findings after being able to interpret their data visually. They noticed certain anomalies in the experiment's setup. One observation was that the water flow actually hit the sample directly, while it was intended to flow over the mineral. Another anomaly they noticed was that the walls seemed to cause the mineral to stick, rather than to flow freely. They additionally noticed the buildup of concentration in low-velocity areas.

Significance & Future Work

Recently, limestone has become a popular choice as an aggregate material for concrete mixtures. With calcite being the main mineral in the composition of limestone, these tests aid researchers in understanding how newer concrete mixtures may react to water flow scenarios. This testing has the potential to inspire newer forms of limestone-aggregate concrete that is more adaptable to water.

Acknowledgements

Special Thanks to:

Steven Satterfield,
Nicos Martys,
and Judith Terrill

References

[1] Braen, D. (2017, June 28). Crushed Limestone Uses & Benefits. Retrieved July 30, 2019, from https://www.braenstone.com/crushed-limestone/

[2] Feng, P., Ye, S., Martys, N. S., & Bullard, J. W. (2020). Hydrodynamic factors influencing mineral dissolution rates. Chemical Geology, 541, 119578. doi: 10.1016/j.chemgeo.2020.119578