The Gap between Visualization Research and Visualization Software (VisGap) (2022)
C. Gillmann, M. Krone, G. Reina, T. Wischgoll (Guest Editors)

Visualization Ecology Applications for Measurement Science: A Visualization Gap Approach

S. Su W. Sherman S. Satterfield T. Griffin S. Ressler W. George S. Feng and J. Terrill

National Institute of Standards and Technology, USA

Abstract

Advanced visualization research have remained insufficiently included in science and engineering workflows due to the highly specialized task-specific requirements and lack of suitable applications. Although the field of visualization is maturing and researchers have invested efforts into introspection and methodologies, much of the research is not readily available to the scientists and engineers in their daily workflow. In our effort to address the visualization gap, we are working to adapt and extend an existing open-source visualization framework in our workflow to streamline our basic research into visualization application to address measurement uncertainty challenges. In addition to benefiting scientists in our organization, we also hope that our contributions to the open-source framework will benefit our customers, the broader scientific community and society.

CCS Concepts

• ***Human-centered computing*** → ***Visualization systems and tools;***

1. Introduction

Advanced visualization research, if applied properly, offers tremendous potential to advance data analysis for scientists and engineers. Together with immersive technologies, advanced visualization techniques offer an increasing opportunity to express scientifically meaningful results. At the National Institute of Standards and Technology (NIST), we are working to advance measurement science by creating a virtual laboratory to interactively measure and analyze scientific data through visualization and immersive technologies [TGG*09].

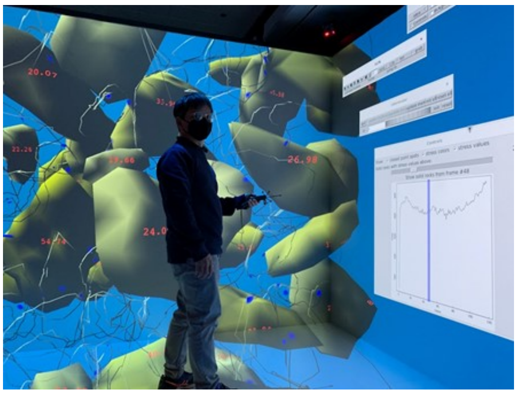

Figure 1: *Measuring Concrete Flow Stress.*

The virtual laboratory shifts the normal activities that scientists perform to understand their data into a virtual environment. Data at NIST spans a wide topical range from nano to cement and other models that exhibit complex dynamics. The virtual environment is our computational laboratory that combines the qualitative with the quantitative as shown in Figure 1. We use visual representation, interactive selection, quantification, and display ecology to portray numerical information from each dataset we visualize. Our virtual laboratory illustrates this approach with a variety of interfaces from immersive to desktop environments that demonstrate the methods used to obtain quantitative knowledge interactively.

Within our virtual laboratory, visualization of complex data and supporting trusted decision making are often challenging. In addition, as standards and technologies evolve, exploring new technological frontiers is also crucial in the development of our virtual laboratory. As data at NIST spans a wide range, multi-modal and high-dimensional data visualization techniques would be needed to visualize data. Human factors and usability are also of particular importance for the virtual laboratory as the resulting scientific measurement can influence the development of NIST products, such as standard reference materials. Furthermore, we provide equity in access to science promoting universally interpretable analysis.

Our virtual laboratory research activities include building on and enhancing an existing open-source software tool that runs on a desktop environment as well as in an immersive environment. We investigate the use of immersive visualization as a scientific instrument for exploration and representation of data while developing

DOI: 10.2312/visgap.20221057

interactive measurement techniques based on visualizations. In addition, we are also developing ways to merge analysis with visualization and provide quantitative feedback into the visualization while exploring and expressing uncertainties due to the data as well as the visualization methods.

One of the main challenges in the development of our virtual laboratory is similar to the major issues encountered in the development of the Virtual Hydrology Observatory project [SCNHG09], VRFire project [SPS*07], and Taverns project [SSHD06]. In all the projects, 3D interactive visualization of High Performance Computing (HPC) generated and/or observed data were primarily used to visualize the outcome of a computer simulation. The ability to gather quantitative measurement from the experiments in an immersive environment were challenging, which can be attributed to a combination of factors including the scaling factor of the data in a virtual environment, the precision and resolution of the interaction techniques supported, and overall user perception of the experiment in a virtual environment compared to the experiment in the real environment.

These challenges cannot be solved using existing visualization tools and often require developing new visualization techniques or incorporating the most recent advancement from the larger visualization community into our solution. In one of our projects, we collaborated with the larger research community to adapt a bivariate glyph design to reveal atom spin behaviors for quantum simulation at NIST [ZBG*16]. Therefore, finding ways to bridge the gap between visualization research and visualization software (VisGap) is crucial in our virtual laboratory development to advance measurement science.

2. Related Work

Research related to visualization ecologies have been building up to our virtual laboratory for scientific workflow development. We believe all the lessons learned from all our previous research are crucial in our ongoing development at NIST to address the visualization gap.

In our virtual laboratory for scientific workflow development, it is unlikely that a single visualization technique will be able to address all data analysis and visualization requirements. Supporting collaborative visualization work benefits from multiple visualization methods as illustrated in our work on large high resolution visualization [SPC*16] [SAP*18], hybrid immersive and non-immersive visualization [SAPC18] [SPD19], and visualization ecology [KBR*19]. We also demonstrated the use of immersive and non-immersive technologies in the development of scientific workflow for scientists and engineers at DEVCOM Army Research Laboratory [SPB*20].

Our past work includes a long history of developing and contributing towards the Open Source software for immersive visualization as demonstrated with our Immersive Plugin for ParaView [SCC*11] and FreeVR [SCS13].

3. Efforts to address Visualization Gap Challenges at NIST

On January 18th, 2022, the Department of Energy (DoE) Advanced Scientific Computing Research program held a workshop on Visualization Grand Challenges for Scientific Discovery, Decision-Making, and Communication. One of the grand challenges discussed during the workshop was the difficulty of measuring visualization-related benefits for practicing scientists and building scientists' trust in the visualization while analyzing the data. At NIST, we are also working on addressing the same research challenges in a cross-disciplinary team. However, addressing this grand challenge and cultivating trust in the visual analytics workflow requires a cross-disciplinary collaborative effort from both visualization scientists and the domain scientists.

The effort to build a successful virtual laboratory will need to leverage all the recent advancements in visualization research. However, with regard to this workshop's main theme – applying basic research results to benefit scientists' research domains – applying new visualization research is not yet a streamlined process. Our existing development demonstrates the significant effort needed to apply visualizations (in particular, visualizations that can easily shift from desktop to immersion) that contribute to the research effort. Therefore, we have begun the work to improve a NIST applied research workflow by streamlining our visualization framework and address the visualization gap by enabling basic research development and applied research efforts to operate within the same framework.

3.1. Building NIST Scientific Workflow based on Open Source Software

As part of our research on Virtual Measurements and Analysis, the Applied and Computational Mathematics Division (ACMD) High Performance Computing and Visualization Group (HPCVG) operates a fully immersive visualization environment (IVE) and has developed high end visualization (HEV) software, based on DIVERSE [KASK02], to run it. Development of this software for our IVE began more than two decades ago. During this period, we have upgraded and rewritten this software as our understanding scientific visualization in an IVE developed and as outside innovations in hardware appeared. However, there are many limitations to maintaining in-house software. For example, HEV could only run on a specially configured operating system, and it had not kept up with recent advances in hardware visualization capabilities – internally it is built on a third party scene-graph framework. Our IVE is on a critical path for the success of collaborations with several NIST research groups and is used at every stage of these collaborations. These projects are diverse and span applications from nanotechnology to medical devices to materials, and often contribute to standard reference data and materials. For example, the IVE was essential in the success of NIST's development of standard reference materials (SRMs) for the measurement of the flow of cement paste, mortar, and concrete. The next step in our software progress has begun by shifting from HEV to ParaView, a fully open source software tool, which includes techniques that take advantage of modern visualization hardware.

The ParaView software system is complex. Internally it uses a pipeline and proxy-based framework to enable multi-system parallel computations. The software consists of a Qt interface which uses over 2000 VTK C++ classes to produce visualizations. It runs in an IVE as well as on Windows, Mac OS X, Linux, SGI, IBM Blue Gene, Cray and various Unix workstations, clusters and super-computers. It supports rendering shaders. It has a new real-time path-tracing back end using NVIDIA RTX technology. Overall, ParaView extends the environments that the HPCVG HEV can work in, plus provides access to real time ray tracing and global illumination now possible with modern GPUs. We started our work on immersive visualization with ParaView by developing an immersive plugin for ParaView extending ParaView to support immersive and non-immersive visualization [SCC*11]. Access to high-end GPU rendering will continue to grow as ParaView adopts the ANARI rendering standard from the Khronos Group [SGA*22].

Our transition to ParaView includes translators that make use of data created by our existing projects, so ongoing projects can make a smooth transition. This year we completed the SAVG (NIST/HEV internal format) reader plugin for ParaView, and an utility to convert the thousands of NIST SAVG format files to the subset defined for the SAVG plugin. In addition, in collaboration with Kitware Inc. (the maintainers of VTK and ParaView), we also completed an OpenXR option to the OpenVR plugin in ParaView to bring it into compliance with the Khronos standard. This creates a uniform interface across all Extended Reality (XR) displays so there is a common software environment across hardware.

We have also begun the development and are currently testing the preliminary support for different frames-of-reference to ParaView. This will enhance ParaView's scene graph capability. We will also create a translator from our HEV timeline files to the ParaView time animation system. Our present HEV timeline methodology is built on a sequence of time deltas with changes in location, orientations and scale that together create a path through a visualization. Interspersed throughout a timeline file are SAVG commands. These SAVG commands can alter the visualization by changing the visibility of parts of the visualization, or recording an image snapshot at a particular time – snapshots can then be merged into an animated movie file. Incorporating these features into ParaView will provide the capability to rerun a visualization session.

Finally, we developed a low-cost hardware methodology that enables the use of consumer VR tracking. This is accomplished by using existing open-source tools along with consumer 6-DOF position tracking systems such as the HTC/Valve Corp "Lighthouse" system. With these tools, collaborators working without the benefit of a full CAVE system can still work with the full user interface of a CAVE benefiting both development and deployment of the immersive visualization features.

3.2. Contributing to Standards in Visualization

NIST joined the Khronos Group last year to contribute to software and data standards that relate to high performance computing and standard and immersive visualization. Researchers from HPCVG are participating members of several software standards working groups, including OpenXR, ANARI, 3D Commerce, and glTF.

For OpenXR, the membership of the Khronos OpenXR working group has continued to grow and includes all of the prominent companies working in the consumer extended reality (XR) arena. This past year new consumer software releases have reflected the growing adoption of this standard through a shift away from hardware-dependent interfaces. This standardization is important as the number of available consumer products in the XR space continues to grow.

NIST, and the ACMD HPCVG in particular, participate in OpenXR working group events as we continue to evaluate the standard for use in internal projects. Indeed, as part of the *"Transition to Open Source Visualization Software"* effort described in the previous subsection, we are collaborating with Kitware Inc. to enable their ParaView scientific visualization tool to operate using the OpenXR API.

Presently, the primary OpenXR focus has been toward head-mounted display (HMD/headset) systems, but as a goal of OpenXR is to be completely display agnostic, the HPCVG group will be bringing its expertise in large-format, CAVE-style displays such as the NIST Immersive Visualization Environment (IVE).

For ANARI, the ANARI (Analytic Rendering Interface for Data Visualization) API is an effort led by the Khronos Group to provide a common library interface for the rendering of scientific data. In particular, ANARI provides a consistent interface for volumes, point clouds and polygonal mesh data that can be rendered using different methodologies, and tuned to the available graphics rendering hardware. This can be rasterized on a CPU-based system, or ray-traced renderings on an RTX-level GPU, or anywhere in between.

In the past year the ANARI standard has been released as a provisional 1.0 specification, with the anticipation that the final 1.0 API will be released in the Summer of 2022. One of ACMD's contributions to the ANARI effort has been to integrate it with the CAVE IVE display system to ensure that the specification is amenable to needs of virtual reality rendering.

In addition, the ParaView scientific visualization tool, is also adopting the ANARI API for its advanced rendering output.

4. Future Work and Discussion

While basic visualization research is a crucial aspect of building useful data visualizations, interdisciplinary collaborations are needed to successfully apply the research into a scientific workflow that a domain scientist can use on a regular basis. All parties in the workflow development should be equally vested in the final outcome of the project. At NIST, computer scientists across disciplines collaborate closely in the development of the scientific workflow.

In addition to the research effort within our division, there are separate efforts within NIST involving collaborations with the larger visualization research community. These collaborations work to develop visualization techniques specifically to address NIST's broad data analysis and visualization challenges. However, to address the visualization gap, the proven basic research development will also need to be applied to the day to day scientific workflow of the domain scientist – and to that end, HPCVG is working to incorporate its expertise in immersive environments into standard tools that also work on the desktop, such as ParaView.

4.1. Enhancement to Open Source visualization framework, ParaView

Our overall approach to bridge typical desktop analysis with immersive systems, such as the NIST IVE, has been to extend the immersive capabilities of an already popular desktop visualization tool. The first step of this effort enabled tracked-perspective multi-screen rendering coupled to the desktop view. The second step has been to integrate the HMD/headset style of XR with the burgeoning OpenXR standard. And next, we are working to enhance the CAVE interactions within ParaView to take advantage of new multi-frame-of-reference capabilities that (through our collaboration with Kitware Inc.) have recently been added to the underlying ParaView rendering system. Support for multiple frames-of-reference help with the bridging of desktop to CAVE-style large immersive systems.

One of our research group collaborators at NIST uses the WRF file format in their atmospheric research. Thus, within our collaboration with Kitware, we are working on a native WRF file format reader for ParaView. This enhancement will eliminate the post processing steps presently needed to transfer atmospheric data from the simulation into ParaView – allowing scientists to perform data analysis on their data without the intervention of the visualization team. ParaView's client-server parallel processing mode will further enhance their workflow by enabling them to directly load their large WRF data files generated on the HPC system into ParaView. (Thus saving transfer time and storage bottlenecks that would otherwise reduce efficiency.) ParaView can then be quickly used on the HPC filesystem for post-processing and visualization. In addition, the scientist can easily transition to working immersively through ParaView's CAVE-interaction plugin, or the XR-interface plugin for HMDs.

4.2. Collaborating with Practicing Scientists to Develop Scientific Workflow

Another within-NIST collaboration of the HPCVG involves working closely with the additive manufacturing group to develop a multi-functional, data-intensive, artificial intelligence (AI)-driven, virtual reality-enhanced laboratory for metal part defect detection and remedy. The goal of this collaboration is to develop a set of visualization tools and a data repository to explore the complex issues of detecting defects from images, physics-informed numerical models, and AI-driven models for modeling and monitoring metal transformation from raw material to products. This collaborative effort includes a development of a new type of laboratory that allows researchers to combine 3D immersive visualization with those use physics-based models, etc.

Through the interdisciplinary collaborations, visualization scientists and the researchers will work together to develop a collaborative scientific workflow that will support visual analytics of large manufacturing and part quality data collected from both experiments and computations. This workflow will also enable accessing the resultant big data and displaying it in the visualization ecology currently in development within HPCVG. With a specific set of requirements from the collaborators, the visualization ecology will support collaborative exploration and validation of computational and experimental data during the knowledge discovery process. Furthermore, the scientific workflow will also support collaborative exploration of research data regardless of the users' geographical locations supporting a post-pandemic hybrid working arrangement.

The Collaborative Virtual Laboratory (CVL) in the new era of AI is intended to address the visualization of big data analytics and measurement uncertainty challenges. It will enable collaborative assessment of the large amount of experimentally collected and/or computationally generated scientific data that may contain subtle information including defects, features, attributes, etc. New method and efficient workflow to analyze, explore and understand the collected research data is extremely important for scientific advancement. The development of this new scientific workflow constitutes a cross-disciplinary innovation requiring close collaboration between scientists from diverse disciplines. In this case, NIST scientists from various technical domains will be working closely with the immersive visualization scientists to provide the necessary systems needed to develop CVL. It is envisioned that the outcome of this project can be integrated into the measurement science daily workflow. Other NIST scientists will have access to CVL advanced scientific workflow that is tailored specifically to address their unique data analysis and knowledge exploration challenges supporting their cutting-edge research activities.

Although the initially developed scientific workflow is custom-tailored to the additive manufacturing and fabricated parts effort, the new competency can be generalized to perform analysis of other areas by adding support for different data types and the development of additional visualization techniques. This expertise will benefit other NIST researchers (like the computational scientists working on atmospheric simulation), NIST's external customers, the scientific community and society while supporting NIST mission.

5. Conclusions

Addressing the visualization gap challenges as highlighted by this workshop will require the combined efforts from the whole community. At NIST, several groups are also working to address some of the same challenges and it is our intention to contribute to those efforts by making our work available to the community. Thus far we have made significant progress through our work building the immersive visualization portion of our scientific workflow – we continue to enhance the CAVE-Interaction interface within ParaView. Our ongoing collaboration with Kitware ensures that these efforts will be pushed out to the ParaView open source community. We are also looking to engage the larger visualization community working on the same visualization gap challenges to collaborate and to shape our ongoing research efforts.

6. Disclaimer

Certain commercial equipment, instruments, or materials (or suppliers, or software, ...) are identified in this paper to foster understanding. Such identification does not imply recommendation or endorsement by the National Institute of Standards and Technology, nor does it imply that the materials or equipment identified are necessarily the best available for the purpose.

References

[KASK02] KELSO J., ARSENAULT L., SATTERFIELD S., KRIZ R.: Diverse: a framework for building extensible and reconfigurable device independent virtual environments. In *Proceedings IEEE Virtual Reality 2002* (2002), pp. 183–190. doi:10.1109/VR.2002.996521. 2

[KBR*19] KOEHLER C., BERGER A., RAJASHEKAR R., WISCHGOLL T., SU S.: Dynamic collaborative visualization ecosystem to support the analysis of large-scale disparate data. In *2019 IEEE International Conference on Big Data (Big Data)* (2019), pp. 3968–3977. doi:10.1109/BigData47090.2019.9006500. 2

[SAP*18] SU S., AN M., PERRY V., JIA J., KIM T., CHEN T.-Y., LI C.: Visually analyzing a billion tweets: An application for collaborative visual analytics on large high-resolution display. In *2018 IEEE International Conference on Big Data (Big Data)* (2018), pp. 3597–3606. doi:10.1109/BigData.2018.8622183. 2

[SAPC18] SU S., AN M., PERRY V., CHEN M.: Realtime interactive hybrid 2d and 3d visual analytics on large high resolution display and immersive virtual environment. In *2018 IEEE 11th Workshop on Software Engineering and Architectures for Real-time Interactive Systems (SEARIS)* (2018), pp. 1–8. doi:10.1109/SEARIS44442.2018.9180229. 2

[SCC*11] SHETTY N., CHAUDHARY A., COMING D., SHERMAN W. R., O'LEARY P., WHITING E. T., SU S.: Immersive paraview: A community-based, immersive, universal scientific visualization application. In *2011 IEEE Virtual Reality Conference* (2011), pp. 239–240. doi:10.1109/VR.2011.5759487. 2, 3

[SCNHG09] SU S., CRUZ-NEIRA C., HABIB E., GERNDT A.: Virtual hydrology observatory: an immersive visualization of hydrology modeling. In *The Engineering Reality of Virtual Reality 2009* (2009), McDowall I. E., Dolinsky M., (Eds.), vol. 7238, International Society for Optics and Photonics, SPIE, pp. 114 – 121. URL: https://doi.org/10.1117/12.807177, doi:10.1117/12.807177. 2

[SCS13] SHERMAN W. R., COMING D., SU S.: FreeVR: honoring the past, looking to the future. In *The Engineering Reality of Virtual Reality 2013* (2013), Dolinsky M., McDowall I. E., (Eds.), vol. 8649, International Society for Optics and Photonics, SPIE, pp. 47 – 61. URL: https://doi.org/10.1117/12.2008578, doi:10.1117/12.2008578. 2

[SGA*22] STONE J. E., GRIFFIN K., AMSTUTZ J., DEMARLE D., SHERMAN W., GÜNTHER J.: Anari: A 3d rendering interface standard. *Computing in Science and Engineering* (2022). doi:10.1109/MCSE.2022.3163151. 3

[SPB*20] SU S., PERRY V., BRAVO L., KASE S., ROY H., COX K., R. DASARI V.: Virtual and augmented reality applications to support data analysis and assessment of science and engineering. *Computing in Science and Engineering 22*, 3 (2020), 27–39. doi:10.1109/MCSE.2020.2971188. 2

[SPC*16] SU S., PERRY V., CANTNER N., KOBAYASHI D., LEIGH J.: High-resolution interactive and collaborative data visualization framework for large-scale data analysis. In *2016 International Conference on Collaboration Technologies and Systems (CTS)* (2016), pp. 275–280. doi:10.1109/CTS.2016.0059. 2

[SPD19] SU S., PERRY V., DASARI V.: Hybrid 2d and 3d visual analytics of network simulation data. In *2019 IEEE International Conference on Big Data (Big Data)* (2019), pp. 3992–3999. doi:10.1109/BigData47090.2019.9006235. 2

[SPS*07] SHERMAN W. R., PENICK M. A., SU S., BROWN T. J., HARRIS F. C.: Vrfire: an immersive visualization experience for wildfire spread analysis. In *2007 IEEE Virtual Reality Conference* (2007), pp. 243–246. doi:10.1109/VR.2007.352491. 2

[SSHD06] SU S., SHERMAN W., HARRIS F., DYE M.: Taverns: Visualization and manipulation of gis data in 3d large screen immersive environments. In *16th International Conference on Artificial Reality and Telexistence–Workshops (ICAT'06)* (2006), pp. 656–661. doi:10.1109/ICAT.2006.122. 2

[TGG*09] TERRILL J. E., GEORGE W. L., GRIFFIN T. J., HAGEDORN J. G., KELSO J. T., OLANO M., PESKIN A. P., SATTERFIELD S. G., SIMS J. S., BULLARD J. W., DUNKERS J. P., MARTYS N. S., O'GALLAGHER A., HAEMER G.: Extending measurement science to interactive visualisation environments. In *Trends in Interactive Visualization* (2009), Liere R. Adriaansen T. Z.-S. E., (Ed.), Springer, London, pp. 287–302. doi:https://doi.org/10.1007/978-1-84800-269-2_13. 1

[ZBG*16] ZHAO H., BRYANT G. W., GRIFFIN W., TERRILL J. E., CHEN J.: Validation of splitvectors encoding for quantitative visualization of large-magnitude-range vector fields. *IEEE Transactions on Visualization and Computer Graphics 23*, 6 (2016), 1691–1705. doi:10.1109/TVCG.2016.2539949. 2