AI-Powered ParaView for NIST: Enabling Accessible Scientific Visualization

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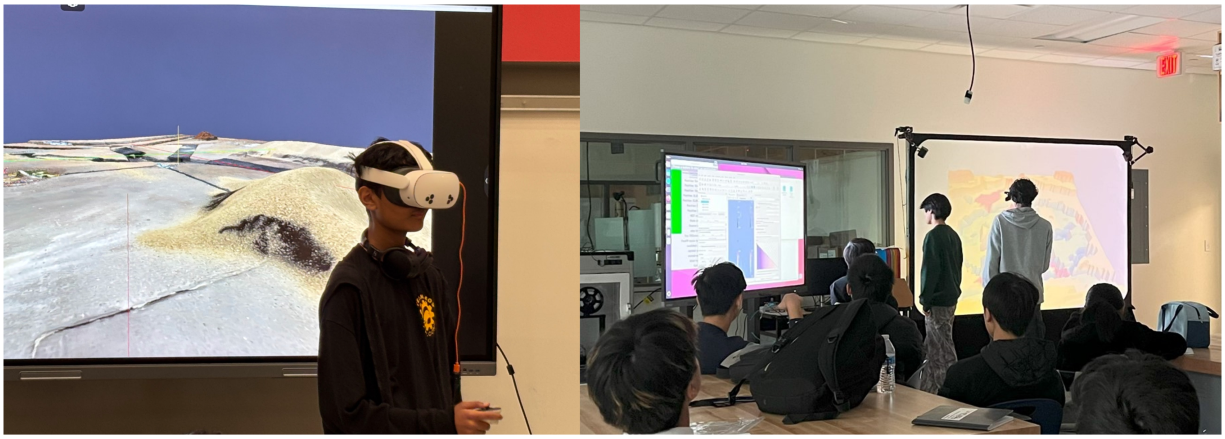

Figure 1: Visualization of a physical model exoplanet using immersive ParaView. On the left, a student is using the ParaView XR Interface Plugin to perform a virtual walkthrough of an exoplanet model using a head mounted display. On the right, a group of students are exploring various geographical features of the exoplanet on a portable single-screen immersive visualization system using the ParaView CAVE Interaction Plugin.

Abstract

This position paper outlines the research agenda for National Institute of Standards and Technology (NIST)'s AI-Powered ParaView effort and how the research directly addresses and supports multiple action items within the America's AI Action Plan. How this project fits within NIST's existing generative artificial intelligence (GenAI) tooling infrastructure and the integration of the AI-Powered ParaView interface will also be described. We propose a set of benchmarks for objectively evaluating AI-Powered ParaView's performance, capabilities, and effectiveness. Additionally, to foster a deeper understanding of GenAI's benefits in scientific data exploration and visualization, we are proposing collaborative projects between NIST's visualization and scientific research communities.

Index Terms: Immersive Visualization, Generative AI.

1 Introduction

Immersive Visualization has tremendous potential as a visual analytics tool for data exploration and discovery[8][3]. The High-Performance Computing and Visualization Group in the Applied and Computational Mathematics Division at National Institute of Standards and Technology (NIST) has long championed immersive visualization to distill meaning from the increasingly complex datasets generated by researchers at NIST (and elsewhere). Our enhancements to ParaView XR Interface Plugin and CAVE Interaction Plugin[7] in the most recent release of ParaView[6] is helping to bridge the "visualization gaps"[9], ranging from high school students to the larger scientific community with visualization software for immersive data exploration as shown in Fig. 1. Our effort to enhance ParaView with immersive visualization functionalities is strategically motivated to maximize the impact of our work to the broader scientific community. Yet, despite successfully lowering the software requirement for immersive visualization with immersive ParaView, the inherent complexity of ParaView as a scientific visualization tool can still present a challenge for wider immersive visualization adoption at NIST.

The steep learning curve of ParaView creates a significant "visualization gap," hindering widespread adoption and delaying discovery. Recent developments in generative artificial intelligence (GenAI) have enabled agentic systems that can now be used to address this visualization gap to promote wider adoption of immersive visualization. The U.S. AI Action Plan[1] has over 30 tasks associated with NIST and we are working on pillars within the action plan to take advantage of the recent development in GenAI.

This short position paper proposes a novel tooling framework by leveraging existing GenAI infrastructure and autonomous agents integrated via the Model Context Protocol (MCP) to make advanced scientific visualization universally accessible to all NIST researchers. We detail the fundamental problems of current visualization bottlenecks and articulate the profound potential impact on accelerating scientific discovery, democratizing visualization, and setting a new paradigm for human-AI interaction for the scientific community at NIST and beyond.

2 Research Agenda

The scientific community generates large and increasingly complex datasets in the advancement of metrological sciences. However, data analysis and knowledge discovery workflows to gain actionable insights from data often require a sophisticated visual analytics process. While scientific visualization tools like ParaView re-

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duce the need for custom graphical programming, there remains a learning curve before mastery of these tools. Researchers, particularly those not specialized in visualization, face extensive training to learn the complicated user interfaces, and expansive filter functionalities. This ”visualization gap” means data often remains under-explored, and the full potential of insight extraction from experimental and simulation results goes unrealized.

Our research addresses this critical challenge by developing “AI-Powered ParaView”. Building on the success of a recently deployed GenAI[2], our goal is to revolutionize how scientists interact with their data, making high-fidelity scientific visualization truly accessible to all.

This research will further democratize high-end visualization by integrating advanced AI, specifically Large Language Models (LLMs), with ParaView through the Model Context Protocol (MCP) and empower researchers to describe their visualization needs using natural language. For example, a researcher can simply state *”Show me the temperature field with an isosurface at 300 Kelvin and color by pressure,”* and the AI agent will translate and apply this request into precise ParaView commands. This shifts the focus from tool mastery to scientific inquiry and acceleration of scientific discovery.

This research will also be establishing “A Paradigm for Future Scientific Tools”. Our work represents a pioneering effort in integrating advanced AI agents with complex scientific software. It is not just about making ParaView easier to use, it's about fundamentally transforming the scientific visualization paradigm, enabling a new era of intuitive, efficient, and insight-driven data exploration, thereby directly enhancing researchers' scientific output and impact.

This effort addresses a core problem in data analysis: the ”visualization gap” – i.e. the gap between the complexity of advanced scientific visualization tools like ParaView and the ease of use required by the broader scientific community.

Our technical plan unfolds in two distinct phases: 1) ensuring a robust foundation, before 2) progressively adding intelligent capabilities; ultimately culminating in a transformative tool for scientific community.

In the first phase of the research, we will be continuing the work by Liu[4] and adapt the current ParaView-MCP to run on an on-premises chat client[2], using the Open WebUI AI platform[10] and the Llama 4 Maverick[5] model instead of the Claude LLM in Liu's implementation. As our modifications will be contributed back to the open-source repository, the resulting integration of ParaView-MCP with Open WebUI will further promote Open-Source adoption. In addition, as we are actively developing new ParaView capabilities, we need to use our own version of ParaView instead of the generic ParaView installed through the Conda package manager.

Also, within the first phase, we will identify the 10 to 20 most commonly used data visualization functionalities as part of enabling AI adoption while helping to develop AI enabled science. Using LLM-based AI will directly address the ”steep learning curve” by pre-packaging essential ParaView operations into easily callable AI tools, making them more accessible to researchers.

As ParaView was not originally designed for integration with agentic systems, we will further develop the multi-client server functionality used by Liu's current implementation to ensure maximum interoperability. This will enable simultaneous interaction by both human users (via the ParaView GUI) and the GenAI (via MCP) within a single ParaView session. This integration is crucial as it enables collaborative visualization: allowing researchers to refine AI-generated visualizations manually or to guide the AI with real-time feedback, thus supporting the broader goal of augmenting expert workflows, furthering enabling AI adoption.

In the second phase, we will conduct a limited deployment, evaluating user engagement, and system capabilities/shortcomings through survey-based experimentation. This will involve integration with a production testing environment similar to a GenAI system currently deployed at NIST. This activity is to seamlessly integrate the ParaView-MCP into this testing environment, resulting in a fully integrated, secure, and performant AI-Powered ParaView service within that environment. This integration directly provides a concrete solution for making AI-powered scientific visualization accessible to scientific research community.

We will also establish quantitative and qualitative metrics for success, with the deliverable being a comprehensive framework for collecting user feedback and system performance data to build an AI evaluation ecosystem. This data will be vital for guiding continuous improvement and identifying areas for future research, providing concrete evidence of addressing the ”visualization gap” and informing future development cycles.

This two-phased approach ensures a robust and progressively increasing intelligent capabilities to culminate in a transformative tool for the scientific community while also working to advance the science of AI.

3 Benchmarks

For this GenAI scientific visualization capability deployment, we propose to objectively measure the system's efficiency in empowering the scientific community with advanced visual analytics capability (bridging the “visualization gap”). In addition, the benchmarks should demonstrate practical utility, AI capabilities, and impact on the scientific workflow of the community.

In the first phase of the research, a simple questionnaire will be circulated to the broader scientific community to gather information on their scientific data analysis workflow. A list of data visualization and data analysis tasks will be compiled from the questionnaires with 10 to 20 of those supported by ParaView being prioritized for initial ParaView-MCP implementation. Those tasks not currently supported by ParaView will also be compiled to inform our ongoing ParaView development.

In the second phase, our research will develop a more comprehensive questionnaire to evaluate the system's efficiency in bridging the “visualization gap.” The data visualization and data analysis tasks compiled from the initial phase will be used to formulate task-specific questions that shape the questionnaires for phase two. This stage will be followed by a more general questionnaire to evaluate practical utility, AI capabilities, and impact on overall scientific workflow.

4 Tooling Infrastructure

Fig. 2 shows the interrelationships between Open WebUI, ParaView-MCP and ParaView. Liu in his paper[4] describes in detail the implementation of ParaView-MCP with the Claude LLM desktop interface. In our implementation, we will replace the Claude LLM desktop interface with Open WebUI and utilize Open WebUI's MCP, MCPO. This decision is based on the fact that the current GenAI implementation at NIST is also built upon Open WebUI. Using this setup, we will expand Liu's ParaView-MCP implementation[4] based on our research and seamlessly deploy our version of ParaView-MCP on NIST's GenAI platform.

Our initial exploration to move from the Claude LLM to Open WebUI is hampered by Python package compatibility issues. Liu paper[4] notes their ParaView-MCP implementation utilizes Python 3.10, with ParaView 5.13.3 installed via the Conda package manager, which also uses Python 3.10. Our project aims to use Python 3.12, which appears compatible with all our various package dependencies. However, a key technical challenge remains: the Python 3.12 environment must be specifically configured to correctly recognize and interact with our ParaView's Python environment. This ensures that the Python 3.12 interpreter can properly import and execute ParaView's modules and functions.

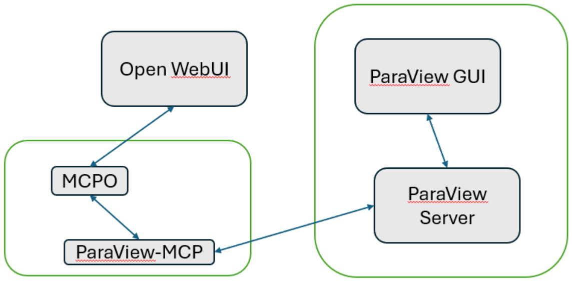

Figure 2: System Architecture of AI-Powered ParaView for NIST. This diagram depicts the system's core components: Open WebUI (user interface) connects to MCPO (Open WebUI's Model Context Protocol), which interfaces with the ParaView-MCP server. The ParaView-MCP server then communicates directly with the ParaView Server for visualization processing. The ParaView GUI also connects to the ParaView Server, enabling multi-client, collaborative human-AI visualization.

Although our system is designed around open-source software, there is of course an accompanying AI-accelerated hardware requirement needed to run our own open-source LLM models. In the current stage of research, the specific graphics hardware requirements are unclear when working with larger datasets within ParaView with the MCP interface. However, there are other parallel efforts in ParaView development that can be leveraged to enable ParaView to take advantage of the same AI hardware for visualization.

5 Collaborative Projects

Our exploration of Liu's implementation[4] on the Claude LLM shows great promise in the use of AI-powered ParaView to close the visualization gap at NIST. Our participation in the current Open WebUI based GenAI agent pilot study at NIST has demonstrated tremendous value in augmenting the non-visualization expert workflow test cases. The implementation of AI-powered ParaView with the existing NIST GenAI agent will put high-end visualization tool in the hand of novice visualization users while raising the quality of visualization tool usage.

Although our AI-powered ParaView platform is turning everyone into a visualization tool expert, it is also a visualization research platform. We will be able to explore automatic selection of the best visualization technique based on prior visualization scenarios or certain characteristics in the data make the user a true visualization expert. By analyzing the visualization techniques employed in successful efforts (as reported via questionnaires), we can incorporate aggregate insights back into the system, offering data-driven recommendations and continually improving best practices.

Beyond ParaView-MCP, Liu in his paper[4] also demonstrated the interoperability between different visualization software tools, such as integrating Blender-MCP with ParaView-MCP. Our effort can expand on this idea to include MCP implementations for other visualization software and allowing the GenAI agent to select which visualization tool will best visualize the particular data enhancing the analysis process.

6 Discussion

This research has the potential for significant and far-reaching impacts across NIST and potentially the broader scientific community. These impacts address the core problems outlined in the proposal and underscore the research's importance.

This research will help accelerate scientific discovery and foster innovation. The research will reduce time-to-insight by significantly lowering the barrier to using advanced visualization tools, allowing researchers to generate, refine, and interpret scientific data much faster. This use of GenAI will also deepen data exploration by providing a more intuitive interface to encourage researchers to explore their data more thoroughly, uncovering subtle patterns, correlations, and phenomena that might have been overlooked due to the complexity of traditional tools.

This work also serves to democratize and broaden the adoption of advanced visualization by empowering non-visualization experts to use more advanced tools. Thus, the most immediate impact will be on researchers who are not visualization experts. They will gain access to high-end visualization capabilities without needing extensive training in ParaView's complex user interface or even more complicated Python scripting. This will empower a much wider cohort of scientists to perform their own sophisticated data analysis.

7 Conclusion

The "visualization gap" represents a pervasive challenge in modern data-intensive scientific research, hindering efficient knowledge discovery. Our proposed research into "AI-Powered ParaView at NIST" directly addresses this bottleneck at the institutional level by pioneering a novel approach to scientific visualization based on GenAI and autonomous agents. The robust tooling infrastructure centered on the MCP and the power of an LLM running locally, aim to transform ParaView into an intuitively accessible data visualization and data analysis tool for the scientific community.

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Certain commercial equipment, instruments, or materials (or suppliers, or software, etc) 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.

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