

# PUBLIC SUBMISSION

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**Comment On:** NSF-2025-OGC-0001-0001  
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## Submitter Information

**Organization:** ParaTools, Inc.

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## General Comment

See attached file(s)

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## Attachments

An AI Software Ecosystem for Scientific Innovation SUBMITTED

## An AI Software Ecosystem for Scientific Innovation

### A Response to the Request for Information on the Development of a 2025 National Artificial Intelligence (AI) Research and Development (R&D) Strategic Plan

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In this RFI response<sup>2</sup>, we<sup>3</sup> address two topics:

*AI research for accelerating fundamental scientific discovery and technological breakthroughs in areas where private-sector investment is insufficient, infrastructure support for the AI research and development community*

In this response, we outline considerations for the next-generation software ecosystem that will support scientific applications integrating AI and more traditional equation-based modeling & simulation (ModSim) to provide a unified AI/ModSim software ecosystem.

#### Key Points:

1. The scientific computing community needs a cohesive AI/ModSim software ecosystem that is vendor neutral, compatible across major vendor platforms, and updated.
2. Public investments in a unified AI/ModSim community ecosystem are important for efficient and effective scientific progress and complement private-sector investments.

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## **A Cohesive Software Ecosystem for AI and Modeling & Simulation**

The next-generation scientific software ecosystem must provide a cohesive portfolio of libraries and tools that facilitate AI and ModSim approaches. As scientific research becomes increasingly interdisciplinary, scientists require both toolsets to address complex, data-rich problems. A unified software ecosystem integrating established AI frameworks and emerging scientific AI frameworks alongside established ModSim libraries is important for solving these next-generation scientific challenges effectively.

## **Leveraging Current Efforts: DOE Efforts in Software Stewardship**

The US Department of Energy laboratories and collaborating partners have sponsored significant software stewardship and advancement efforts, especially in the post-Exascale Computing Project (ECP) era, to provide long-term support for libraries and tools used by the DOE and broader community in advanced computing. These efforts include funding for math, data and visualization, performance analysis, and programming systems libraries and tools, as well as for curating a portable, reliable, and performant version-compatible portfolio of these libraries and tools and their dependencies. While the current DOE-supported ecosystem includes many AI libraries and tools that our scientific community needs, installing the comprehensive AI ecosystem is challenging and labor-intensive, especially on high-performance computing (HPC) systems. The PESO Project<sup>4</sup>, led by the authors of this document and their laboratory collaborators, is one of the projects involved in post-ECP efforts, sponsoring efforts to expand the use of the popular scientific software package management, Spack<sup>5</sup>, in open-science codes and to curate and deliver E4S<sup>6</sup>, the software ecosystem created by ECP.

## **Developing a Consistent and Evolving Software Ecosystem**

Providing a consistent and up to date software ecosystem that incorporates AI and ModSim software libraries and tools will require significant effort in identifying the core requirements, converting those requirements to specifications and design, and producing a cohesive software ecosystem that is easily used in a portable way and available with significant updates on a regular schedule that users can count on. While present AI users are typically using industry-provided capabilities that target a broad spectrum of domains, we anticipate the creation and wide use of AI libraries and tools specifically trained for

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<sup>4</sup> Heroux, Michael A., et. al. "PESO: Partnering for Scientific-Software Ecosystem Opportunities." 2024. [PESO Project Website](#)

<sup>5</sup> Todd Gamblin, Matthew P. LeGendre, Michael R. Collette, Gregory L. Lee, Adam Moody, Bronis R. de Supinski, and W. Scott Futral. [The Spack Package Manager: Bringing Order to HPC Software Chaos](#). In *Supercomputing 2015 (SC'15)*, Austin, Texas, November 15-20 2015. LLNL-CONF-669890.

<sup>6</sup> Heroux, Michael A., et al. "E4S: Ecosystem for Science." 2021. [E4S Website](#)

scientific problems. These libraries and tools must be curated and provided to the scientific community, especially on leadership computing platforms.

### **Need for a Portable and Cohesive Library and Tool Ecosystem**

Traditionally, computing system vendors have provided these kinds of libraries. However, insufficient effort has been applied to making a portable and cohesive library and tool ecosystem that users can rely on, independent of which vendor's platform they are running on. The Exascale Computing Project made progress in providing a portable, high-performance software ecosystem that provides libraries and tools for established ModSim applications for users on major HPC platforms. The same basic approach needs to be explored for high-performance, portable software solutions on the growing variety of AI for science computing platforms. *While computer system vendors such as NVIDIA and AMD are invested in providing software ecosystems for their users, the community can benefit from an industry effort that is not tied to any specific hardware platform. In collaboration with system vendors and the Department of Energy, independent scientific software companies can play an important role in this effort.*

### **A Unified Framework for AI and ModSim Software**

The complexities of managing AI and ModSim software products go beyond supporting individual libraries and tools products and highlight the need for DOE to support efforts that bring AI and ModSim libraries and tools into an integrated ecosystem. This approach is particularly important when ensuring compatibility across different versions of programming systems (for example, different Python and C++ standards), hardware platforms, and performance requirements. This integrated approach would allow scientists to seamlessly combine AI and ModSim capabilities, leveraging the strengths of both to address next-generation scientific problems more effectively.

### **Conclusion and Recommendations**

By supporting a cohesive, integrated portfolio of AI/ModSim scientific tools and libraries, we can facilitate more rapid development, greater collaboration across domains, and efficient scaling of AI/ModSim techniques to new scientific discoveries. We believe continued investments in community-driven ecosystems like the Ecosystem for Science (E4S) and Spack can bridge the AI and ModSim communities by providing standardized, flexible, and performance-optimized environments that integrate AI and ModSim software.