Cover Letter for the 2025 PESO Project Report

January 2026

Partnering for Scientific-Software Ecosystem Opportunities (PESO)

Dear Reader,

We are pleased to share the 2025 PESO Project Report with you. Science increasingly depends on powerful computers and the complex software ecosystems that support them. From large-scale simulation and data-intensive discovery to emerging AI-driven workflows, scientific software is essential to advancing knowledge, innovation, and national priorities. The PESO Project exists to strengthen this software foundation to support scientific discovery.

PESO advances the U.S. Department of Energy's scientific software ecosystem by coordinating stewardship, integration, and quality-focused activities across a diverse portfolio of DOE-funded software projects. Working in close partnership with the Consortium for the Advancement of Scientific Software (CASS), PESO focuses on ecosystem-level challenges—such as interoperability, sustainability, and usability—while complementing the product-level stewardship provided by individual software teams and by other software stewardship organizations, our CASS partners. Our collaborative model brings together experts from national laboratories, universities, and industry to ensure that scientific software can be assembled, validated, and sustained in practice.

In 2025, in collaboration with CASS partners, PESO's efforts emphasized:

- **Strengthening software ecosystem coordination and integration**, reducing fragmentation across libraries, tools, and workflows, and improving interoperability on current and emerging DOE computing platforms.
- **Advancing E4S and Spack** as foundational ecosystem products, delivering curated, version-compatible software portfolios with ecosystem-level validation to support both traditional high-performance computing (HPC) workloads and AI-enabled scientific workflows.
- **Improving software quality, security, and sustainability**, including expanded integration testing, adoption of best practices, and rollout of a CASS-wide Impact Framework to support transparent stewardship and continuous improvement.
- **Enhancing user and developer experience**, making scientific software easier to adopt, deploy, and use effectively through improved documentation, usability research, and community-shared resources.
- **Building and sustaining the scientific software community**, through leadership in CASS, contributions to the High Performance Software Foundation, workforce development activities, and continued investment in community resources such as BSSw.io and the Better Scientific Software Fellowship Program.

Through these activities, PESO helps prepare the DOE scientific software ecosystem for evolving computing environments, including accelerator-dominated systems, cloud-adjacent platforms, and AI-integrated workflows aligned with DOE's Genesis Mission. By addressing software challenges at the ecosystem level, PESO enables researchers, facilities, and vendors to focus more effectively on scientific outcomes and time to discovery.

We invite you to explore the full report. We hope it conveys both the scope of PESO's work and the importance of sustained, coordinated investment in scientific software as critical infrastructure for science.

Sincerely,
The PESO Project Team

PESO Project Report 2025

PESO: Partnering for Scientific-Software Ecosystem Opportunities

January 2026

U.S. DEPARTMENT of ENERGY | Office of Science

PESO Project Report 2025

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1 Executive Summary

The PESO Project advances the scientific software ecosystem for the U.S. Department of Energy (DOE) Office of Advanced Scientific Computing Research (ASCR) by supporting and coordinating activities that enable DOE-funded scientific software to function as a coherent, sustainable ecosystem. Through collaborations within the Consortium for the Advancement of Scientific Software (CASS), PESO provides shared infrastructure, coordination, and stewardship practices that improve interoperability, quality, and adoption across a diverse portfolio of scientific libraries and tools. These activities are designed to complement, not replace, product-level stewardship by individual teams and software stewardship organizations (SSOs).

High-level funding summary. The PESO Project's annual budget is $4M, supporting 40 staff members at 8 DOE labs, four industry partners, and one university. By design, many PESO team members also receive funding from partner SSOs, enabling close coordination and reducing duplication of effort across the CASS portfolio. Approximately 75 percent of PESO's budget supports cross-SSO collaborations:

- **Technical collaborations**: Approximately 54% of PESO funding supports technical collaborations that strengthen interoperability, testing, and infrastructure among SSOs.
- **Spack and E4S**: 25% of PESO funding provides direct support for Spack and E4S, the two cornerstone PESO software products that deliver and curate the DOE Office of Science's software portfolio.
- **Community and outreach collaborations**: Rougly 21% of PESO funding supports community and outreach collaborations that promote visibility and broad adoption of DOE scientific libraries and tools, as well as workforce development.

CASS collaborations: Technical activities related to scientific software. PESO collaborations strengthen the interoperability, quality, and sustainability of DOE scientific software through joint work with CASS member SSOs that focus on software products in applied math (FASTMath); AI, data, and visualization (RAPIDS); programming models and runtimes (S4PST), and tools for performance and correctness (STEP). Advances in FY25 addressed software ecosystem definition and integration, continuous integration (CI) and complementary testing, software quality assurance, impact measurement, and user-developer experience.

CASS working groups led or staffed by PESO personnel—including the Software Ecosystem, Integration, and Impact Framework groups—developed shared definitions, impact measures, and workflows that allow DOE software to interoperate efficiently and evolve coherently. These collaborations support DOE advanced computing facilities (ALCF, NERSC, OLCF) by improving software deployment coordination and streamlining ecosystem-level CI testing. In FY26, these groups will extend work to deploy the new Impact Framework, expand OpenSSF and GoodDocs quality efforts, and strengthen cross-facility engagement.

PESO software products. About a quarter of PESO's resources focus on two key deliverables that anchor the DOE scientific software ecosystem:

- **Spack**: Delivered and supported for DOE Office of Science facilities and software teams, Spack achieved its 1.0 release in FY25, marking a milestone in reproducibility and binary cache management. PESO ensures ongoing maintenance, CI capacity, and community engagement through HPSF, where Spack is now a core project. Subsequent releases (v1.1 and v1.2) addressed facility-specific challenges such as compiler mixing and expanded binary compatibility.
- **E4S**: PESO curates a broad portfolio of DOE Office of Science libraries and tools, ensuring version compatibility and publishing verified Spack recipes. FY25 advances included GPU runtime integration for NVIDIA, AMD, and Intel platforms; expanded AI/ML tool support; and containerized E4S releases in AWS, Google Cloud, and Adaptive Computing Cloud environments. FY2026 priorities include CI modernization, enhanced documentation, and improvements to container usability.

Together, Spack and E4S operationalize the DOE software ecosystem by providing a coherent distribution, validation, and delivery pipeline for hundreds of scientific software products.

CASS collaborations: Community and outreach activities. Community-oriented collaborations extend the reach and sustainability of DOE's software ecosystem. PESO supports leadership for the CASS Steering Committee and multiple working groups, while also staffing a range of cross-SSO initiatives that cultivate the scientific software workforce and public visibility. Highlights from FY25 include:

- The **Better Scientific Software (BSSw)** program, which published over 40 new articles on bssw.io and awarded the 2025 BSSw Fellowship cohort
- **Outreach activities** such as the HPC Best Practices Webinar Series and tutorials at ATPESC and SC conferences, reaching more than 1,400 participants
- Engagement in the **High Performance Software Foundation (HPSF)**, which welcomed Microsoft and ARM as new members and held its first HPSFCon in May 2025, with over 200 attendees

In FY26, PESO and CASS will continue these outreach and workforce efforts, expand participation in HPSF, and launch new initiatives such as the Scientific Software Horizons podcast series—all with the goal of advancing the scientific software ecosystem as needed for next-generation scientific discovery.

2 Introduction

Science increasingly depends on powerful computers and their complex software ecosystems that integrate applications, libraries, tools, workflows, and deployment technologies across diverse computing architectures. These ecosystems underpin advances across nanomaterials modeling, energy systems, data-driven discovery, and AI training. Ensuring that this software can be assembled, validated, and sustained in practice is therefore essential to scientific progress.

The PESO Project [99] advances the scientific software ecosystem for the U.S. Department of Energy (DOE) Office of Advanced Scientific Computing Research (ASCR) by coordinating stewardship, integration, and quality-focused activities across DOE-funded software projects. PESO focuses on strengthening today's software collections through ecosystem-level processes, shared infrastructure, and cross-project coordination, while also anticipating future computing environments. This work includes preparing simulation and data-centric software to support emerging AI-driven workflows—such as equation-based components required for advanced AI world models—aligned with DOE's Genesis Mission [117].

Through collaborations within the Consortium for the Advancement of Scientific Software (CASS) [40]*, PESO provides shared infrastructure, coordination, and stewardship practices that improve interoperability, quality, and adoption across a diverse software portfolio. These activities are designed to complement, not replace, product-level stewardship by individual teams and software stewardship organizations (SSOs).

This PESO Project Report summarizes the achievements and impact of the project from inception in Fall 2023 through December 2025†, discussing both PESO software products and collaborations in CASS with other SSOs on technical activities related to scientific software as well as community and outreach activities. As shown by the PESO organizational chart in Figure 1, the PESO team, by design, includes members of partner SSOs focused on software product stewardship (FASTMath [53], RAPIDS [103], S4PST [105], and STEP [110]), who serve as liaisons to software product communities to engage these groups in advancing the scientific software ecosystem, with an emphasis on integration and software quality as needed for next-generation scientific discovery. We also partner with representatives from the National Nuclear Security Administration (NNSA), funded separately but engaged as team members to better ensure consistency and complementarity, as both ASCR and NNSA invest in and leverage open-source products such as Spack.

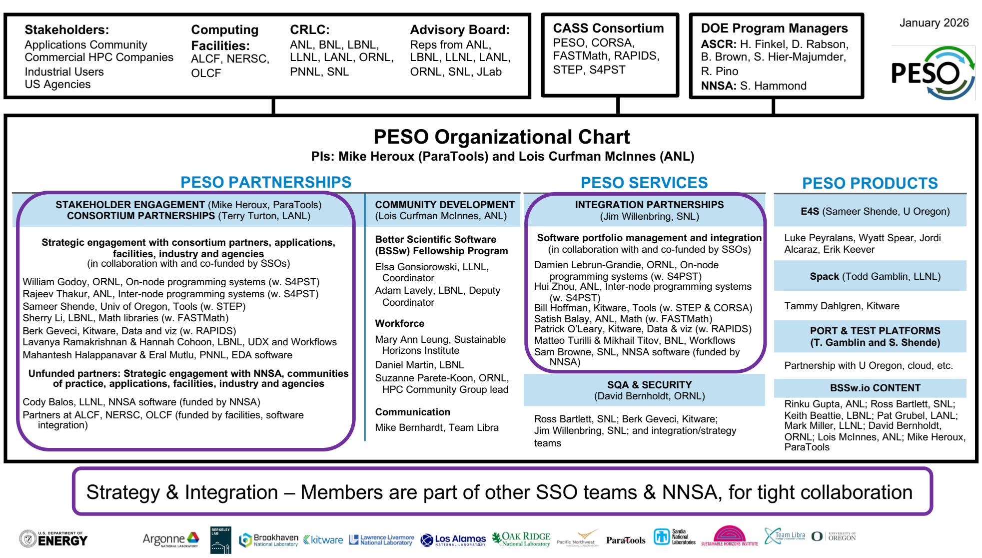

Figure 1: *This team chart illustrates PESO partnerships, services, and products that advance the scientific software ecosystem in collaboration with other SSOs through CASS and the broader community. PESO's staffing strategy intentionally co-funds staff who are also funded by other SSOs, facilitating coordination and communication across teams.*

*Section 5.1 introduces CASS and PESO's roles within the consortium.

†The 2024 PESO Project Report [71] provides additional details of 2024 achievements.

Background and history. The foundation of the PESO team and strategy is our collective insight and community connections over decades of research and development in scientific computing, most recently with PESO PIs (Heroux and McInnes) leading the Software Technologies focus area [43, 57, 69, 87] and the IDEAS productivity project [88] of the DOE Exascale Computing Project (ECP) [42, 79], and PESO staff leading and developing a wide range of premier scientific libraries and tools [72, 74]. Each member of the PESO team has extensive experience in advancing scientific software products and development practices, while serving as community leaders as we embrace next-generation challenges in high-performance computing (HPC) and AI [1, 17, 73, 75, 86, 97, 111].

Budget overview. Figure 2 provides FY25 budget information, considering focus areas and institutions.

Label	Focus Areas	Budget ($K)	Category Total ($K)	Collaborating Institutions
Technical Topics: CASS Collaborations			**$2,165**	
T1	Software Ecosystem	$475		ParaTools, ANL, Kitware, LBNL, LLNL, LANL, ORNL, PNNL, SNL, UOregon
T2	Integration: Product families	$490		SNL, ANL, BNL, Kitware, LBNL, LLNL, LANL, ORNL, ParaTools, PNNL, UOregon
T3	Integration: Crosscutting	$450		SNL, ANL, BNL, Kitware, LBNL, LLNL, LANL, ORNL, ParaTools, PNNL, UOregon
T4	Impact Framework	$150		ORNL, ANL, Kitware, ParaTools, SNL
T5	Software Quality Assurance	$390		ORNL, ANL, BNL, Kitware, LBNL, PNNL, SNL, UOregon
T6	User and Developer Experience (UDX)	$210		LBNL, ANL, Kitware, ORNL, ParaTools
PESO Software Products			**$1,000**	
P1	E4S Enhancements and Adoption	$500		Univ of Oregon
P2	Spack Enhancements and Adoption	$500		LLNL, Kitware
Community and Outreach: CASS Collaborations			**$835**	
C1	CASS Consortium	$120		ANL, LANL, ORNL, ParaTools, SNL
C2	Community Development	$495		ANL, LBNL, LLNL, LANL, ORNL, ParaTools, SHI, SNL
C3	HPSF	$70		LLNL, Kitware, ORNL, ParaTools, SNL, UOregon
C4	Outreach	$150		ANL, ORNL, LANL, ParaTools, Team Libra
	Total		**$4,000**	

(a) PESO budget by focus areas

Institution	Staff, Travel, M&S	Focus Area Contributions
ANL	**$756,200**	T1, T2, T3, T4, T5, T6, C1, C2, C4
Univ of Oregon (joint appt)	$100,000	T1, T2, T3, T5, C3
ParaTools (project leadership collaboration)	$305,000	T1, T2, T3, T4, T5, C1, C2, C3, C4
Univ of Oregon (E4S)	$500,000	P1
Team Libra (communication)	$13,800	C4
LBNL	**$280,000**	T1, T2, T3, T5, T6, C2
SHI (community development)	$60,000	C2
LLNL	**$416,659**	T1, T2, T3, P2, C2, C3
Kitware (Spack)	$163,341	P2
ORNL	**$415,000**	T1, T2, T3, T4, T5, T6, C1, C2, C4
Kitware (software ecosystem and integration)	$400,000	T1, T2, T3, T4, T5, T6, C3
BNL	**$150,000**	T2, T3, T5
LANL	**$140,000**	T1, T2, T3, C1, C2, C4
PNNL	**$50,000**	T1, T2, T3, T5
SNL	**$250,000**	T1, T2, T3, T4, T5, T6, C1, C2, C3
Total	**$4,000,000**	

(b) PESO budget by institutions

Figure 2: **(Left)**: *This table summarizes the PESO budget. CASS technical collaborations (involving partner SSOs) on technical activities account for 54%. Advances in E4S and Spack account for 25% of the PESO budget (or $1,000K annually) and contribute to foundational software ecosystem capabilities. Community and outreach collaborations account for 21%. In total, 75% of the PESO budget (or $3,000K annually) funds PESO-CASS-SSO collaborations.* **(Right)**: *The PESO partner institutions collaborate on the various PESO focus areas. This table summarizes PESO institutional budgets and contributions to focus areas, using the labels (T1, C2, and so on) introduced in the left-hand table.*

The remainder of this report provides information on each PESO focus area, with emphasis on CASS collaborations, achievements, impact, and future plans.

3 Technical Topics: CASS Collaborations

PESO's collaborations on technical topics focus on five complementary thrusts: software ecosytem (Section 3.1), integration (Section 3.2), impact framework (Section 3.3), software quality assurance and security (Section 3.4), and user and developer experience (UDX) (Section 3.5).

3.1 Software Ecosystem

Software ecosystem overview and CASS coordination. The PESO Software Ecosystem thrust defines, coordinates, and operationalizes a coherent scientific software ecosystem spanning individual product efforts of other SSOs within CASS. We address ecosystem-level concerns, including portfolio composition, integration boundaries, lifecycle alignment, and shared stewardship expectations. PESO leads and significantly staffs the CASS Software Ecosystem Working Group (WG) [36], which provides a forum for cross-SSO coordination among FASTMath, RAPIDS, S4PST, STEP, CORSA, and PESO. This WG works closely with other CASS working groups, including Integration, Impact Framework, and SQA, to ensure ecosystem concepts are consistently reflected across technical and community activities.

Since October 2023, Software Ecosystem activities have increasingly incorporated forward-looking considerations related to cloud-native computing and AI-enabled workflows. These discussions are informed by emerging DOE system directions, including AI-factory-style platforms and hybrid on-prem/cloud usage models, and by PESO-led ecosystem vision discussions that explore the convergence of AI and modeling and simulation software. We are also tracking emerging software ecosystem needs for quantum computing. Coordination with other CASS working groups ensures that these forward-looking perspectives are grounded in practical stewardship considerations rather than treated as standalone shifts.

Addressing the needs of scientific computing communities and contributing to DOE's mission. Software Ecosystem efforts address the needs of scientific computing communities by reducing fragmentation and uncertainty as software stacks evolve to support new workflows, architectures, and execution models [2, 26, 29, 30, 31, 32]. Scientific applications increasingly rely on combinations of tightly coupled simulations, ensemble workflows, data-centric pipelines, and AI-based components. Without ecosystem-level coordination, these trends can lead to duplicated effort, inconsistent deployment, and barriers to adoption.

Engagement with DOE computing facilities—including ALCF, NERSC, and OLCF—has been an important input to this work. Through regular interactions, targeted discussions, and informal ”teatime” sessions, facilities have highlighted both near-term operational concerns and longer-term trends, such as the growing importance of elastic resource usage, interruption tolerance, and data-driven workflows. Even for on-prem systems, cloud-native environments and practices are becoming increasingly relevant due to architectural diversity, accelerator dominance, and integration with AI workflows.

The Software Ecosystem thrust also contributed to two recent community reports [86, 97] and a PESO-led document on cohesive AI and modeling and simulation software stacks [70]. This document situates cloud-native considerations such as containerization, workflow orchestration, data provenance, and service-oriented access as part of a broader ecosystem evolution rather than a replacement of traditional HPC. Collectively, these activities support DOE's mission by preparing the software ecosystem to sustain scientific productivity as computing platforms and usage models diversify.

Priorities if increased funding were available. Software Ecosystem efforts would prioritize deeper engagement and broader participation over scope expansion alone. A priority would be more structured engagement with application teams and facilities to better understand how cloud-native practices, AI-assisted workflows, and accelerated architectures influence software requirements. This could include pilot activities that connect ecosystem concepts to concrete application and facility use cases.

Additional funding would also support stronger integration between the Software Ecosystem WG and other CASS working groups to address emerging lifecycle questions, such as how applications transition toward service-oriented or workflow-centric deployment models, and how stewardship expectations should evolve as codes incorporate AI components or operate across on-prem and cloud environments. Finally, increased resources would enable further development and dissemination of ecosystem vision and guidance documents, helping the DOE scientific software community anticipate and adapt to long-term shifts toward cloud-aligned, data-centric, and AI-integrated computing paradigms.

3.2 Integration

Integration overview and CASS coordination. The PESO Integration thrust focuses on efforts at the levels of scientific software ecosystem and individual product communities, including on-node and inter-node programming systems, tools, data and visualization, math libraries, and workflows. The goals are to improve quality, sustainability, delivery, and interoperability across the ecosystem. The dual focus on ecosystem and product levels is essential given the challenges of creating a cohesive ecosystem that includes product communities with diverse needs and varying levels of maturity.

A common objective across integration initiatives is to move activities, where appropriate, to higher levels to improve efficiency. For example, we can transfer some testing from the product community to the ecosystem level and eliminate redundancy in porting efforts. The overarching goal is to continue improving the interoperability, delivery, and quality of the software technologies ecosystem developed under ECP, emphasizing community efforts and incorporating new technologies as needed by next-generation science.

Coordination with CASS SSOs is intentionally built into the integration thrust. Core integration team members are associated with STEP, S4PST, RAPIDS, and FASTMath (see Figure 1). Integration planning activities are aligned with the planning of the partner SSOs. This approach facilitates the use of best practices and injects an explicit focus on quality and sustainability into efforts across the ecosystem, making possible activities that could not be supported by the partner SSO alone, and improving many others. The result is that a large majority of integration efforts are collaborative with another SSO and/or software product team.

Addressing the needs of scientific computing communities and contributing to DOE's mission. Integration efforts within PESO address a core need of scientific computing communities: the ability to rely on complex software stacks that function correctly, perform as expected, and evolve without disrupting downstream users. Ecosystem-level integration testing plays a central role in building and sustaining trust in DOE software investments. By testing collections of libraries and tools together—rather than in isolation—PESO integration activities help identify compatibility issues early, before they reach application teams or facility users. This approach improves software quality by exercising codes across a variety of hardware architectures, compilers, and configurations, enabling errors to be detected and addressed upstream.

Communal integration resources, particularly the Frank [116] CI platform at the Univ. of Oregon,[‡] reduce overall cost while expanding access to advanced testing capabilities. By providing shared CI infrastructure with diverse CPU and GPU resources, PESO enables CASS projects to conduct testing that would be impractical for individual teams to maintain independently. This shared model aligns with DOE's mission by improving software readiness for leadership computing facilities and reducing redundancy.

PESO integration activities have produced several concrete outcomes that reflect user and facility expectations. The team developed initial Spack environment templates for DAV (Data, Analysis, and Visualization) and Tools that capture commonly expected functionality, along with optimizations and extensions relevant to DOE platforms. PESO supported interoperability across a broad set of ecosystem packages, including Kokkos, Viskores, ADIOS2, ParaView, and xSDK member packages. Notable achievements included transitioning Viskores to C++17, enabling HIP/ROCm support on Ascent, and formalizing DAV Spack builds across Frontier, Aurora, and Perlmutter. Additional efforts included supporting FASTMath xSDK release activities, adding Spack packages for workflow tool dependencies, and partially supporting an eScience'25 workshop focused on workflows [68] and a DOE SULI [106] intern. PESO also supported early development of the Build-pulse tool [101], which aggregates and analyzes Jenkins build logs across large CI workloads; while still under development, this tool is already being used to support preparation for the MPICH 5.0.0 release. The DOE RECUP project further leveraged PESO guidance on SDK best practices when establishing its repository structure, illustrating cross-project knowledge transfer within CASS.

[‡]The Frank CI platform was established during the DOE Exascale Computing Project; no PESO funding supports equipment.

Promoting best practices for coding, sustainability, maintenance, and support. PESO integration work promotes best practices by embedding quality, sustainability, and maintainability considerations directly into shared testing and release workflows. A significant portion of this work focused on supporting product integration testing, particularly in coordination with DAV and Tools stakeholders. The team maintained and evolved DAV and Tools environments to track advancements in underlying software, including Viskores, ADIOS2, Catalyst, DIY, HDF5, Ascent, ZFP, ParaView, HPCToolkit, PAPI, and TAU, as well as dependent packages such as VisIt and VTK. These efforts ensured that integration environments remained representative of current user expectations while avoiding stagnation.

Several activities addressed sustainability and technical debt. PESO helped reduce technical debt in Kokkos CI workflows, standardized results reporting, and configurations, and hardened integration testing pipelines. The team also supported modernization of the Kokkos release process to better serve a growing user base, including improvements to maintain consistency between Kokkos and Trilinos and the addition of tests to preserve interoperability with dependent codes. Complementary efforts contributed tools that assist Kokkos users in porting applications to newer releases and supported improvements in Kokkos packaging, including Kokkos assuming ownership of relevant Spack packages and clarifying dependency expressions.

Integration efforts also restored and strengthened testing capabilities across several tools, reestablishing nightly and facility testing for TAU and HPCToolkit and adopting the ReFrame testing framework for MPICH. Security and sustainability practices were advanced through leadership in OpenSSF Scorecard adoption. For DAV products, particularly ADIOS2, scorecard improvements raised the score from 7.1 to 8.6 through vulnerability remediation, stricter CI policies, and improved dependency controls. A specific CI vulnerability related to tj-action/changed-files was identified and addressed, and outreach to maintainers of ZFP, DIY, HDF5, and Viskores encouraged similar practices. Parallel efforts initiated OpenSSF Scorecard adoption across multiple Tools components, including Darshan, Dyninst, and HPCToolkit, with PESO providing templates, guidance, and targeted fixes. Across these activities, the team maintained and repaired CI infrastructure, ensured consistent documentation generation via Doxygen and ReadTheDocs, and improved internal knowledge sharing through updated documentation strategies.

Integration mechanisms for bringing new software projects into SSOs and transitioning packages. PESO integration mechanisms emphasize structured onboarding, reproducibility, and clear expectations for ongoing maintenance. New projects are typically onboarded by establishing CI testing and Spack-based builds, enabling them to participate in ecosystem-level validation. Since October 2023, PESO established CI testing on Frank for DIY, Viskores, ParaView, Catalyst, and ADIOS2. Efficiency improvements such as build caching reduced CI overhead, while new components like gh-gl-sync standardized GitHub–GitLab integration. Testing scope expanded to include Python packages and GPU-enabled configurations, with notable advances, such as support for Anari 0.15.0 in Viskores and Python free-threading in VTK, positioning ParaView for improved build concurrency.

Partnerships across CASS further strengthened onboarding pathways. Collaboration with S4PST supported evolution of MPICH CI testing to leverage Spack, substantially reducing build overhead for CI jobs. PESO also worked with FASTMath to highlight CI opportunities on Frank and provided hands-on support for modernizing workflows. These efforts led to improved Spack-based CI pipelines for AMReX, stabilization of PETSc CI, resolution of dependency inconsistencies, and increased confidence in reproducible environments for FASTMath stakeholders. Additional projects are expected to engage in similar improvements. PESO also partnered with the NNSA Integration effort to establish a candidate Trilinos CI build on Frank, with ongoing work toward ROCm support and plans to integrate this build into the Trilinos CI infrastructure within the current fiscal year.

Together, these integration activities illustrate a consistent approach to onboarding, sustaining, and—when appropriate—transitioning software within the CASS ecosystem, reinforcing DOE's investment in reliable, maintainable, and interoperable scientific software.

Priorities if increased funding were available. While the integration effort has made significant progress on several fronts, there is no shortage of work that could be done with additional funds. Specifically, more effort could be applied to getting additional product teams set up to use Frank and setting up and supporting interoperability between products, especially math libraries. Smaller investments would allow more point to point integrations; larger investments would enable better product family and ecosystem level support for the integrations being tested. Another opportunity is workflows, as this area does not have dedicated SSO support. Additionally, more individualized support for best practices could be given to product teams. For example, documentation improvements tend to require some customization per product. Exactly which efforts would be prioritized depends on individual software product needs and would be coordinated with other SSOs.

A significantly underfunded resource is the Frank cluster [116]. While silicon vendors such as NVIDIA, AMD, and Intel provide their latest devices as development resources and charge very little, the infrastructure that supports Frank—the racks and file system in particular—are old and at risk of failure. Given the importance of Frank to our porting and CI testing workflows, we would welcome funds to establish and execute an upgrade plan and the potential to expand support of CI testing to more ASCR projects. Commercial cloud credits (AWS) handle about 60% of the build volume, but they cannot replicate the specialized architecture of DOE Leadership Computing Facilities. The 'Frank' infrastructure is the only testbed capable of validating the exotic hardware configurations required by ASCR's mission. 100% of HPSF [76] CI working group projects' CI is done on Frank. This includes products such as Kokkos, HPCToolkit, ADIOS2, AMReX, WarpX, and Viskores that require GPU access for CI testing. This is the only GPU resource available for HPSF CI.

3.3 Impact Framework

Impact Framework overview and CASS coordination. The Impact Framework (IF) Working Group [28] is a CASS-wide activity led by PESO with additional participation from other PESO staff as well as from all other CASS members. From PESO's perspective, this activity is closely related to the Software Quality Assurance focus area. The IF work also responds to a request from ASCR to develop a common framework across all CASS members by which to track the stewardship activities and progress of the individual software products in the portfolio. The Impact Framework thrust focuses on evaluating scientific libraries and tools to improve their overall impact on scientific advancement and to inform future funding requirements for stewardship. It is a challenging topic area, as libraries and tools can have impacts in many and varied ways, making it difficult to determine a specific framework that is both flexible and fair while also providing a guide for improving the impact and insight into the entire portfolio. Currently, the focus is on exploring ways to measure and improve software and on developing a framework adaptable to a wide range of products. The first version of the Impact Framework [27], has been approved by the CASS Steering Committee and is in the process of being rolled out to the SSOs and their software teams. The plan is to iteratively refine the Impact Framework annually based on feedback and experience.

Addressing the needs of scientific computing communities and contributing to DOE's mission. The core purpose of the Impact Framework activity is to provide a common and transparent vehicle to track software stewardship activities taking place across a portfolio or software ecosystem. Both aspects (commonality and transparency) are essential to our ability to incentivize and reward software improvement processes taking place throughout the portfolio. And improvements in DOE software and in the software development processes used to create and maintain it benefit the computational science and engineering community and further DOE's scientific mission.

Promoting best practices for coding, sustainability, maintenance, and support. The Impact Framework process provides a basis for 1:1 conversations with project teams as to their needs and priorities as they relate to software process improvement. Further, recognizing that individual projects will be in different places regarding their lifecycle and the maturity of their software development processes, the IF approach provides a mechanism to encourage all software teams under a given SSO or the entire portfolio to pursue common goals that can support ecosystem-level goals. For example, CASS leadership might agree that all projects should satisfy certain minimum requirements, such as providing a CITATION.cff file as a clear indication to users of how the software should be cited when it is used, or satisfying the OpenSSF Best Practices "passing" badging criteria. Visibility into planned activities will also allow the PESO Community and Outreach thrusts to develop resources (webinars, BSSw.io [11, 67] content, etc.) on topics being pursued by CASS software products.

Mechanisms for bringing new software projects into SSOs and transitioning packages. One of the intended uses of IF documents completed by stewarded projects is to allow the sponsoring SSO to evaluate whether the stewardship support is being used effectively and providing the desired results, both individually and at the portfolio level. The CASS SSOs may then use the information to guide projects toward activities that are likely to be more useful and effective, or to adjust their stewardship portfolio—potentially phasing out support for projects showing a lower return on investment and bringing in new packages.

Priorities if increased funding were available. We envision three types of activities that could improve the effectiveness and value of the IF thrust if additional funding were available, ordered by the potential for near-term impact. One would be to increase the level of 1:1 engagement with product teams as they define and pursue their stewardship goals (i.e., guidance and coaching). These efforts would naturally connect to the Software Quality Assurance thrust. Second would be to increase the curation and development of resources to address stewardship activities of interest to the product teams (BSSw.io resources, webinars, tutorials, etc.). These efforts would naturally connect to the Community and Outreach thrusts. Third would be an effort to look across the CASS portfolio and the various stewardship activities undertaken from a software engineering perspective to develop a better understanding of what "works" and what doesn't in the scientific software ecosystem. This effort would also naturally connect to the Software Quality Assurance thrust and would be a longer-term activity.

3.4 Software Quality Assurance and Security

SQA overview and CASS coordination. The general goal of the Software Quality Assurance and Security (SQA) area of PESO is to enhance the quality and security of the software in the CASS ecosystem, including work focused on individual packages, across product communities, or even the entire portfolio. We plan to encourage the adoption of impactful SQA goals to build toward common levels of SQA across the portfolio, while respecting teams' individual priorities. The SQA thrust's activities are synergistic with the CASS Impact Framework WG and Integration WG, which have strong participation across CASS SSOs.

Addressing the needs of scientific computing communities and contributing to DOE's mission. Given the direct connection between the quality and trustworthiness of the software and that of the science it enables, anything that improves software quality will contribute to improvements in the reliability of the scientific output, thus benefiting DOE's scientific mission.

Supporting best practices in coding, sustainability, maintenance, and support. Generally speaking, SQA activities focus on supporting and improving software best practices. During FY25, the primary focus of SQA efforts was to lead the CASS Impact Framework WG to agree on a framework [27] that could be used to track SQA-related work across the portfolio and to work with the CASS Metrics WG to help identify a collection of metrics [13] that will be recommended to software teams in conjunction with their Impact Framework planning. In FY26, the SQA team will work through the IF WG to roll out the Impact Framework approach to the stewarded software product teams across CASS and then, individually and through the Integration team, to assist the product teams in implementing their plans. We will also work with the CASS Metrics WG and the CORSA team to identify and collect metrics that will support understanding team progress.

Numerous other SQA-related activities have taken place, with much of the effort carried out by members of the PESO team engaging as part of the Integration thrust. Examples include improvements in CI testing and work toward OpenSSF Best Practices badges. The PESO team led a detailed response to an inquiry from DOE ASCR about the appropriateness of the OpenSSF badging program for the software in the ASCR ecosystem, and presented a webinar on the OpenSSF badging program [3]. Other efforts included prototyping of tools to gather software quality information, such as quantifying results from the clang-tidy static analysis tool for C/C++ code.

Mechanisms for bringing new software projects into SSOs and transitioning packages. There is a general expectation that stewardship support should result in improvements in software quality over time, which might, e.g., be tracked through the Impact Framework effort. Although the specifics of each project will differ, projects that do not appear to be making sufficient progress on SQA improvements over time should be considered by their sponsoring SSO for more intensive oversight and possibly for the redirection of stewardship funding. Individual SSOs or the CASS leadership as a whole may choose to set particular SQA targets for stewarded projects, which could become part of future funding considerations.

Priorities if increased funding were available. There is an additional opportunity related to the "security" element of the SQA thrust, which would be to bolster the resources and training opportunities available related to security concerns in scientific software. For example, the OpenSSF Best Practices badge requires someone in the project to have training in software security. The trainings that OpenSSF offers to satisfy this requirement require a significant time investment (minimum of 18 hours) and do not align well with the concerns of scientific software developers. Many in the CASS community have cited this as a concern or a barrier to obtaining OpenSSF certification for their project. Other topics also are of interest, such as the creation and use of software bills of materials (SBOMs) in scientific software. Additional funding would allow the PESO SQA team to engage with the National Science Foundation (NSF)-funded Trusted CI center [114] to customize their training materials for our community's needs or develop alternative solutions.

3.5 User and Developer Experience (UDX)

UDX overview and CASS coordination. The User and Developer Experience (UDX) thrust area focuses on enhancing the usability, accessibility, and productivity of CASS tools and technologies for end users and developers in service of software stewardship. This thrust area addresses key challenges in improving the interactions and workflows involving HPC software and services, making them more intuitive, efficient, and tailored to the needs of diverse user communities. The PESO UDX thrust achieves this by using established user experience resources and methods (e.g., [12, 84, 85, 93, 94, 95, 102]), sharing knowledge and reusable resources with the community, and through direct collaboration with CASS software teams. This effort is especially critical as AI tools become increasingly part of scientific workflows. By refining user interfaces, improving documentation, and enabling easier deployment, the UDX effort helps ensure that CASS software products are effectively adopted and deliver value to stakeholders. Moreover, by upskilling the staff who create CASS libraries and tools, this thrust trains the community to create more usable software. The UDX efforts in PESO lay a strong foundation for software and usability for broader DOE efforts, including the Genesis mission and its goals of rapid increases in productivity. The UDX thrust will provide software product teams with techniques to identify unseen bottlenecks and frictions that reduce productivity.

Addressing the needs of scientific computing communities and contributing to DOE's mission. The UDX thrust's primary efforts have impacted the E4S project's stewardship through qualitative research to identify usability issues. We carried out E4S stakeholder interviews and conducted an exercise with E4S stakeholders to better understand the value propositions community members perceive from E4S. The UDX thrust also provided heuristic usability evaluations for the CASS and E4S websites to recommend specific changes to improve their design and more effectively convey information. Improving communication will drive adoption of and engagement with DOE software products. As a result of the analysis, the UDX team proposed revisions to have the E4S website better appeal to new users, noted next steps to improve E4S usability, and identified opportunities to facilitate community-based stewardship of E4S.

In partnership with the PESO SQA thrust, we have begun discussions about potentially connecting volunteer technical writers from the Good Docs Project [112] with software teams interested in improving their documentation. This work—an outcome of a CASS UDX webinar [104]—will reduce developers' effort, ensure usability for humans, and streamline the information required to enable AI agents to rapidly interact with and support DOE SC software products. In FY26, we will partner with the SQA thrust to identify and adapt standard user experience metrics to scientific software (particularly HPC and AI) to complement the SQA team's metrics.

Promoting best practices for coding, sustainability, maintenance, and support. The PESO UDX thrust coordinated with the CASS UDX Working Group [38] to organize three webinars in 2025 [14, 104, 108] to highlight best practices and challenges for usable scientific software. Recordings and slides from these webinars are available via the CASS events website [25]. In 2026, we anticipate hosting four to five webinars, one of which has already taken place [115]. In FY26, the PESO UDX thrust will disseminate reusable resources on best practices for developing usable software and onboarding users. Through these curated resources and ongoing webinars, we will empower software developers to recognize and address issues that negatively impact adoption or use. Recognizing the rapid uptake of chatbots and conversational agents, in FY26 we will develop guidance on design best practices for these systems' interfaces in scientific contexts. PESO products like E4S that offer this tooling can leverage UDX recommendations to increase the utility of AI resources to DOE users.

Priorities if increased funding were available. AI tooling is poised to transform the scientific software ecosystem. Software quality, maintenance, and stewardship will be even more critical in this changing landscape. With increased funding, the UDX thrust would explore how AI agents can encourage software stewardship with minimal disruption to established software lifecycle practices. Current information on best practices for agent and chatbot interfaces does not fully encompass the needs of scientific software developers and users. With increased funding, the UDX thrust could identify gaps and propose vital features for AI interfaces in science. Tailoring design best practices to the DOE community's needs would enable the creation of more effective and user-centered AI interfaces for science, helping to accelerate work.

4 PESO Software Products

4.1 E4S

E4S overview and CASS coordination. E4S [46, 120] is one of two core PESO software products serving as an operational realization of ecosystem-level integration within CASS. E4S curates and delivers a version-compatible portfolio of DOE-relevant scientific libraries and tools using Spack-based workflows, with validation through ecosystem-level continuous integration (CI) and interoperability testing. The primary role of E4S is to reduce integration friction across software product families and to provide a tested baseline that complements product-level stewardship conducted by individual projects and SSOs.

E4S activities coordinate with CASS governance and working groups, including Integration, Software Quality Assurance and Security (SQA), Impact Framework, Metrics, and User–Developer Experience. PESO personnel participate directly in these groups, ensuring alignment between E4S curation decisions and broader ecosystem objectives. Thus, E4S serves as a shared integration environment where software stewarded by FASTMath, RAPIDS, S4PST, STEP, CORSA, and PESO can be integrated and tested together under representative configurations that increasingly reflect emerging HPC–AI and cloud-adjacent usage models.

Addressing the needs of scientific computing communities and contributing to DOE's mission. E4S addresses the needs of scientific computing communities by delivering a coherent, tested software portfolio that reflects how applications are assembled and deployed in practice. Application teams and facilities routinely face challenges stemming from complex dependencies, architectural diversity, and evolving workflows. By curating and validating interoperable libraries and tools, E4S reduces redundant integration effort and surfaces ecosystem-level issues earlier in the software lifecycle.

Since PESO began, E4S has introduced numerous new products [50, 51] and expanded its scope to support DOE investments in Electronic Design Automation. E4S Release 25.11 curates 125 primary products and hundreds of dependencies, while tracking emerging trends such as ensemble-based workflows, interruption tolerance, and tighter coupling between simulation and AI pipelines. Although E4S is not a cloud platform, its emphasis on reproducible builds, container-friendly packaging, and portable deployment supports both on-premises and off-premises execution, helping prepare DOE software portfolios for hybrid and cloud-aligned environments without requiring wholesale migration from traditional HPC systems.

These activities improve software readiness and reliability for leadership computing facilities while enabling AI-for-science and data-centric workflows. Facilities and vendors use E4S as a reference integration target to evaluate new architectures and deployment models, reducing risk and time-to-science. As world models increasingly complement large language models in scientific and mainstream AI, the equation-based simulation libraries curated in E4S—executing on modern accelerator-based systems—will remain a critical resource. E4S represents the largest curated open-source collection of such software, and PESO is coordinating with American Science Cloud (AmSC) leaders to ensure emerging AmSC requirements are supported within E4S.

Promoting best practices for coding, sustainability, maintenance, and support. E4S promotes best practices through shared curation, validation, and feedback mechanisms, as well as community policies used to assess product readiness for inclusion in E4S [47]. Ecosystem-level CI testing integrates software under realistic dependency, compiler, accelerator, and container configurations, complementing project-level CI and SQA. This approach is increasingly important as applications adopt more modular, workflow-driven, and ensemble-oriented execution patterns associated with cloud-native readiness.

The E4S website [46] is a core deliverable and the primary documentation and user-support entry point for end users, application teams, facility staff, developers, and vendors. It provides clear orientation to E4S goals, releases, and supported platforms, along with guidance for obtaining and deploying E4S via Spack, containers, or preconfigured environments.

The new E4S Learning Portal [48] supports onboarding, with an initial focus on Summer 2026 DOE lab interns in coordination with mentors and facilities. The E4S Quickstart Guide [52] already provide a parallel environment to new users in a few minutes. The E4S product catalog [49] offers a structured, curated view of the portfolio organized by product family, helping stakeholders understand E4S software.

For contributors, the website documents expectations for package inclusion, quality, and release processes, clarifying how projects fit within the broader ecosystem. Interactive support tools—including prompt-building guides and the E4S Guide Bot—provide AI-assisted navigation of documentation, package discovery, and guidance on installation, configuration, usage, and initial code generation. These features lower barriers for new users while improving efficiency for experienced practitioners, reflecting E4S's emphasis on scalable, ecosystem-level documentation rather than ad hoc, project-specific guidance.

Mechanisms for bringing new software into E4S and transitioning packages. The mechanisms used by E4S to onboard new software are consistent with PESO and CASS integration practices. New packages are typically included after demonstrating technical maturity, relevance to DOE scientific workloads, and the ability to interoperate with other ecosystem components under supported configurations.

E4S also provides a structured framework for portfolio management, including reassessing packages whose relevance, usage, or maintenance status has declined. Information from Impact Framework activities, combined with integration and CI results, provides decision-support inputs for CASS SSOs when evaluating continued stewardship, de-emphasis, or transition of packages. This process supports a coherent, manageable, and defensible stewardship portfolio as ecosystem requirements evolve.

Priorities if increased funding were available. E4S increases would focus on deepening integration and validation capabilities rather than indiscriminately expanding scope. A primary area of emphasis would be targeted expansion of the AI-related portion of the E4S portfolio, coordinated with PESO Integration and SQA activities to ensure interoperability, sustainability, and facility relevance.

Additional resources would also enable expanded CI coverage for configurations that reflect cloud-adjacent and hybrid usage patterns, including more extensive container-based testing, broader GPU coverage, and validation of workflows that emphasize ensembles, restartability, and data movement. These investments align with modernization pathways and would strengthen E4S's role as an ecosystem-level proving ground for software designed to operate across on-premises, hybrid, and cloud-native environments.

4.2 Spack

Spack [54] has become the *de facto* standard for software delivery in the HPC ecosystem and is now used by major supercomputing centers and laboratories worldwide. By providing a unified interface for managing software complexity across laptops, clusters, and leadership-class systems, Spack substantially reduces the effort required for software installation and maintenance and improves software portability across architectures. Developed under the NNSA Advanced Simulation and Computing (ASC) program and adopted as the primary integration tool during the Exascale Computing Project, Spack now serves as a foundational component of the CASS ecosystem and is a founding project of the High Performance Software Foundation (HPSF) [76]. While NNSA supports the foundational development of Spack's core technologies, PESO's investment is distinct and critical: it directs Spack's capabilities toward ASCR-specific integration challenges, open-science facility deployment, and the interoperability required by the CASS ecosystem.

Spack consists of three primary components: (1) a core command-line tool that provides configuration, constraint solving, and user interfaces; (2) a community-maintained repository of over 8,600 package recipes written in a Python-based domain-specific language (DSL); and (3) a cloud-hosted build and test infrastructure that executes over 100,000 builds per week across Amazon Web Services and the University of Oregon Frank cluster [116]. This infrastructure validates changes to package recipes, supports continuous integration, and produces publicly available binary caches. The Spack package repository also serves as the upstream software distribution on which E4S builds.

Under PESO, the Spack project works closely with CASS SSOs to ensure that features required by ASCR software developers are supported in Spack, that package recipes remain functional and interoperable, and that shared CI infrastructure continues to operate reliably. Spack supports sustained software projects across the CASS portfolio, including STEP, S4PST, FASTMath, RAPIDS, and PESO products such as E4S. PESO provides the essential stewardship infrastructure that converts contributions from thousands of DOE scientists into a reliable, tested software stack. Without PESO's ecosystem-level validation, these disparate community contributions would remain fragmented and unusable at leadership facilities.

Addressing the needs of scientific computing communities contributing to DOE's mission. Scientific software is often difficult to configure and deploy on modern HPC and AI systems due to complex versioning, build options, and interdependencies. Applications frequently require specific combinations of libraries and features, and these requirements are not always explicit or easily reconciled. Spack addresses this challenge by providing a domain-specific language for expressing software dependencies and constraints, along with a solver [55] that can construct consistent and compatible software environments on demand.

Under PESO, continued investment in Spack's build and test infrastructure has enabled large numbers of software configurations to be validated with minimal manual effort. The Spack release process has been automated to support both regular and long-term support releases of Spack and its package repository. PESO-supported efforts have also enabled rapid incorporation of new software versions through dozens of package updates, improving software availability and reducing integration effort for DOE facilities and projects. Additional work has focused on improving reproducibility by enabling more consistent sharing of Spack build configurations across sites.

Adhering to best practices for coding, sustainability, maintenance, and support. Given the scale and activity of the Spack community, the project emphasizes automation and policy-driven workflows to ensure sustainability. PESO supports Spack's continuous integration infrastructure, which performs automated builds and tests for releases and enforces a secure binary distribution model. Public binaries are signed and distributed only from reviewed package recipes, while untrusted builds are excluded from distribution.

All contributions to Spack undergo unit testing, recipe audits, and static analysis checks to enforce best practices and detect errors early. Recent improvements include automated verification of artifact checksums and expanded static analysis to detect invalid dependencies and configurations. Spack aligns with OpenSSF security practices and currently satisfies the majority of OpenSSF scorecard checks, with ongoing work to automate remaining requirements.

The project emphasizes continuity across releases through detailed release notes, automated migrations where possible, and backporting of bug fixes, performance improvements, and security updates to long-term support releases. This approach allows users to benefit from reliability and security improvements without requiring frequent major upgrades.

Mechanisms for bringing new software projects into Spack and transitioning packages. Spack emphasizes low-barrier onboarding for both users and contributors. The project provides regular tutorials at major conferences and an annual full-day virtual tutorial, helping users gain confidence in deploying and extending Spack-based environments.

For contributors, Spack provides automated tooling to generate new package recipes, simplified mechanisms for maintainers to manage long-term package ownership, and notification systems that support distributed maintenance. The project actively removes deprecated versions and features from package recipes to control technical debt and maintain long-term sustainability.

Priorities if increased funding were available. The highest priority for expanded Spack support is improving turnkey installation of AI software. While Spack supports major AI frameworks, these are often built from source, whereas users expect rapid installation from optimized binaries. Increased investment would enable expansion of Spack's build cache to provide optimized, architecture-specific binaries for common GPU platforms and DOE systems, allowing faster installation and easier integration of AI and HPC software. Additional priorities include strengthening supply-chain security through automated generation of software bills of materials (SBOMs) and tighter integration with national vulnerability databases. These capabilities would enable more systematic tracking of vulnerabilities across software stacks and reduce reliance on manual, maintainer-driven update processes.

5 Community and Outreach: CASS Collaborations

PESO's community and outreach collaborations consist of work in four complementary thrusts: contributions to the Consortium for the Advancement of Scientific Software (CASS) (Section 5.1), community development (Section 5.2), contributions to the High Performance Software Foundation (HPSF) (Section 5.3), and outreach regarding CASS and scientific software ecosystems (Section 5.4).

5.1 CASS Consortium

The overall CASS goal is advancing scientific software in service of scientific discovery, thus strongly contributing to DOE's mission through coordination and collaboration of member SSOs (currently PESO [99], FASTMath [53], RAPIDS [103], S4PST [105], STEP [110], and CORSA [41]) under the umbrella of CASS.

The PESO-CASS relationship is broad and deep. PESO leaders have invested significant effort in bootstrapping CASS and serving in leadership roles within CASS (see below). Establishing this organizational approach and making it work in the loose federation that is CASS has required careful design and thoughtful implementation. In addition, many of PESO's public-facing activities are CASS-branded, reflecting PESO's role at the ecosystem level and its built-in structural connections to the other SSOs.

CASS community. The CASS leadership team is working to foster a *community organization* (see, e.g., [78]) that fully leverages each SSO and its member projects to ensure strong impact of CASS software products and activities on scientific computing communities. PESO members in CASS leadership roles include:

- **David Bernholdt** (ORNL): Chair of CASS Steering Committee (SC), FY25–26; CASS Impact Framework WG chair, FY25–26; CASS bootstrapping co-lead, FY24
- **Terry Turton** (LANL): Vice Chair of CASS SC, FY25
- **Jim Willenbring** (SNL): Vice Chair of CASS SC, FY26; CASS Integration WG chair, FY25–26
- **Mike Heroux** (ParaTools): CASS Software Ecosystem WG chair, FY25–26
- **Lois McInnes** (ANL): CASS Workforce WG chair, FY25–26; CASS bootstrapping co-lead, FY24
- **Hannah Cohoon** (LBNL): CASS User–Developer Experience WG co-chair, FY25–26

In addition to these formal roles, Jim Willenbring serves as PESO's representative on the CASS Steering Committee, and Mike Heroux and Lois McInnes, as members of the PESO leadership team, have been broadly engaged in CASS leadership activities.

CASS bootstrapping. Shortly after the CASS-affiliated SSOs were established in Fall 2023, we bootstrapped CASS entities. The following timeline shows when CASS governance documents and working groups (WG) were established:

Jun 2024 Impact Framework WG [28] → **Jul 2024** CASS Charter [19] → **Aug 2024** CASS By-laws [18] →
Sep 2024 Metrics WG [34] → **Nov 2024** CASS Steering Committee [37] → **Dec 2024** CASS Website [40] →
Jan 2025 Software Catalog [35], Integration WG [33] → **Feb 2025** Software Ecosystem WG [36] →
Jul 2025 User-Developer Experience WG [38] → **Sep 2025** Workforce WG [39]

Community building and outreach: The CASS Steering Committee has laid the foundation for establishing a CASS External Advisory Board and an HPC Vendor Forum (planned for launch in 2026). In parallel, the CASS community has raised awareness of consortium and SSO activities through multiple venues, including CASS presence at the DOE booth at SC24 and SC25, a lightning talk [9] at the SC24 BOF on *Scientific Software and the People Who Make It Happen: Building Communities of Practice* [5], participation in annual SC events [22], and CASS Community BOF Days in 2024 [23] and 2026 [23]. CASS also organized two minisymposia at SIAM-CSE25 [20, 21], as highlighted in a *SIAM News* article [109]. Additional CASS outreach is discussed in Section 5.4.

5.2 Community Development

PESO's community development thrust encompasses activities to foster a robust community of individuals passionate about scientific software and career paths in developing and using software for scientific discovery. PESO leads the **BSSw.io website** (`https://bssw.io`) [67], a community hub for sharing information on best practices for scientific software development, which published over 40 articles in FY2025 (and similarly in 2018–2024); see highlights for 2024 [65] and 2025 [66]. PESO also leads the **Better Scientific Software (BSSw) Fellowship Program** [10] (partnership among DOE ASCR, NNSA, and NSF) to foster and promote practices, processes, and tools to improve developer productivity and software sustainability of scientific codes. Established by the IDEAS-ECP Project [88], the BSSw Fellowship Program has recognized 38 BSSw Fellows and 38 Honorable Mentions in cohorts 2018–2025; see [15, 59], with emphasis on cohorts during PESO's tenure [60, 61, 63, 64], whose work (made available through bssw.io) includes training on a wide array of topics in formats such as webinars, tutorials, workshops, online training materials, and blog articles. Through a memo of understanding with the US Research Software Engineer Association (US-RSE) [113], we recognized the 2024 [96] and 2025 [80] BSSw Fellowship cohorts at US-RSE'24 [118] and US-RSE'25 [119] and plan to continue in future years. We recently selected the 2026 cohort, consisting of 6 BSSw Fellows and 6 Honorable Mentions, to be publicly announced in early 2026.

PESO members lead the **CASS Workforce Working Group** [39], whose goal is to advance leadership in next-generation computing sciences, with emphasis on robust and innovative scientific software as a cornerstone of advancing basic science, innovation, and security. Prior work [83] and FY25 highlights:

- The **HPC Workforce Community Group**—designed to attract individuals to the scientific software community and promote stable, long-term career paths—hosted several well-attended webinars [58, 98, 121] to promote career paths in scientific computing.
- PESO partially supported the **Sustainable Research Pathways (SRP)** Matching Workshop [82], held online on Dec. 2–5, 2025, with additional support provided by NAIRR [89] and HPSF [76]. SRP pairs lab staff with students and faculty-student teams from various backgrounds in summer internships to foster collaborations and build new pathways to DOE labs. Over 140 participants attended the workshop, including staff from 4 PESO labs (ANL, LBNL, LANL, SNL) who represented 17 projects.
- As requested by DOE ASCR, the CASS Workforce Working Group developed a template and set of **slides highlighting various aspects of workforce and teams** for scientific software, including the impact of student interns hosted by CASS projects through SRP, SULI, and other programs

5.3 High Performance Software Foundation (HPSF)

Launched in May 2024, HPSF [76] is a neutral hub for open-source software for high-performance computing. **Purpose:** HPSF supports the use and sustainment of applications, libraries, and tools in a portable, performant scientific software stack. **Mechanisms:** HPSF promotes and incentivizes improved software quality, availability, and use through collaboration, project mentoring, active working groups, and events (including the first HPSFCon conference in May 2025, the second upcoming in March 2026 [77], and BOFs at various international venues). **PESO contributions:** PESO efforts and resources have been integral to HPSF's growth and execution, including Todd Gamblin (co-founder; Governing Board (GB) Chair; HPSFCon program committee), Damien Lebrun-Grandié (GB; Technical Advisory Committee (TAC); HPSFCon program committee), Bill Hoffman (TAC Chair), Jim Willenbring (TAC), Sameer Shende (TAC), and Mike Heroux (membership recruitment). PESO members (Gamblin, Heroux, Willenbring, Shende) also serve on Technical Steering Committees for HPSF projects including E4S and Spack. **Forward plans:** launch an HPSF CI/CD service with AWS, Azure, and the University of Oregon; participate in CI/CD and Binaries working groups; and expand HPSF participation and activities.

5.4 Outreach

PESO provides planning, coordination, and delivery of CASS-level outreach, such as the development of various CASS impact stories [26, 29, 30, 31, 32] and engaging other CASS member teams to reach the broader community [25]. We also raise awareness of the importance of scientific software libraries and tools in scientific discovery. This outreach is distinct from and complementary to Community Development (Section 5.2), which focuses on growing the scientific software community. Recent highlights include:

- **In-person tutorials on best practices for scientific software** at the Argonne Training Program on Extreme-Scale Computing (ATPESC) [8] and SC25 [4]
- **HPC Best Practices Webinar Series**: produced 6 webinars in 2025 [3, 44, 45, 56, 81, 100], with 1481 total registrants; similarly, produced 7 webinars in 2024, with slides and recordings available via [25]
- **User/Developer Webinar Series**: produced 3 webinars in 2025 [14, 104, 108] with slides and recordings available via [25]
- **SC25 BOF on *Scientific Software and the People Who Make It Happen: Building Our Communities and Practices*** [6], and likewise for SC24 [5, 7]
- **CASS GenAI Scientific Software Teatime** - informal monthly discussion forum launched in 2025

In preparation for 2026:

- **2026 CASS Community BOF Days**: online BOFs on topics related to scientific software [24]
- **Scientific Software Horizons Podcast**: new series planned to launch in early 2026 [107]
- **Intern E4S Tutorials**: Self-paced and interactive content, coordinated with lab mentors [48]

5.5 Impact and Needs

Addressing the needs of scientific computing communities and contributing to DOE's mission. These community and outreach efforts (particularly the BSSw Fellowship Program, BSSw.io, and work by the CASS Workforce Working Group) provide vehicles for engaging talented people with strong skills and interest in high-quality software to learn about DOE scientific computing activities and needs, and to provide pathways for further interactions (e.g., see [63, 64] for insights from BSSw Fellowship cohorts 2023 and 2024 and similar articles by prior cohorts [62, 90, 91, 92]). Thus, these efforts help to address pressing challenges in building the research innovation workforce, while providing creative incentives and rewards mechanisms, and increasing partnerships among academia, national laboratories, nonprofits, and industry.

Promoting best practices for coding, sustainability, maintenance, and support. PESO and CASS community and outreach efforts provide online training materials on effective software practices, which can be used as continuing education for professionals and resources for students. Available through BSSw.io—with contributions from over 345 people, including BSSw Fellows, members of PESO and other SSOs, and the broader community [16]—these resources address the broad scientific software categories of better planning, development, performance, reliability, collaboration, and skills, with topics such as revision control, performance portability, reproducibility, testing, AI for better development, and many others [67].

Priorities if increased funding were available. A priority for increased funding would be a commitment of annual ASCR support for two BSSw Fellows and two Honorable Mentions (which we have been seeking annually from ASCR post-ECP as a separate grant). Having a firm, longer-term commitment from ASCR would enable much-needed stability in the program, complementing similar commitments from NSF and NNSA. Another priority would be modest support for Sandbox Studio, our BSSw.io collaborator.

Increased funding would also enable us to address many emerging needs for expanded training and outreach to address changes in next-generation scientific software ecosystems, particularly the incorporation of AI.

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