# PESO Community Workshop

**Argonne National Laboratory** 

June 8 – 9, 2023



# Toward a Post-ECP Software Sustainability Organization (PESO) Workshop Opening Remarks

- Michael Heroux (Sandia National Laboratories; PI)
- James Ahrens (Los Alamos National Laboratory)
- Todd Gamblin (Lawrence Livermore National Laboratory)
- Timothy Germann (Los Alamos National Laboratory)
- Xiaoye Sherry Li (Lawrence Berkeley National Laboratory)
- Lois Curfman McInnes (Argonne National Laboratory)
- Kathryn Mohror (Lawrence Livermore National Laboratory)
- Todd Munson (Argonne National Laboratory)
- Sameer Shende (University of Oregon)
- Rajeev Thakur (Argonne National Laboratory)
- Jeffrey Vetter (Oak Ridge National Laboratory)
- James Willenbring (Sandia National Laboratories)

Argonne National Laboratory
June 8 – 9, 2023





## Thank you

- DOE ASCR
- Argonne National Laboratory
- Seed Projects Colleagues
- Workshop Presenters
- Attendees
- Writers



Thursday, June 8, 2023			
Topic	Leads	Comments	
Registration / Working Breakfast			
Plenary Kickoff	Mike Heroux (PESO PI)	Give overall workshop charge	
Applications Perspectives	Andrew Siegel (ECP Applications Development Director)	Challenges and opportunities for increased impact of libraries and tools on application success	
Industry Perspectives	Jeff Larkin (NVIDIA), Berk Geveci (Kitware)	Challenges and opportunities for increased impact of libraries and tools in collaboration with industry	
Break			
Advanced Computing Facilities Perspectives	Katherine Riley (ALCF), Balint Joo (OLCF), Richard Gerber (NERSC)	Challenges and opportunities for increased impact of libraries and tools in collaboration with computing facilities	
Set up for breakouts		Describe charge questions, take Q&A, locate breakout rooms	
Lunch			
Lunchtime Talk	Ulrike Yang (ECP xSDK Project PI)	How software product communities can enhance the productivity of teams	
Breakout session			
Break			
Breakouts resume			
Report out from breakouts			
Adjourn		Dinner on your own	
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## Agenda



	Friday, June 9, 2023				
Time (CT)	Topic	Leads	Comments		
7:30 am	Working Breakfast				
8:30 am	Challenges and Opportunities for Computing	Rick Stevens (ANL, Assoc Lab Director, Computing, Environment and Life Sciences)	Roles of sustainable software ecosystems in addressing next-generation computing challenges		
8:45 am	Software Foundations	Todd Gamblin (PESO co-PI)	How we can leverage software foundations for DOE software sustainability		
9:00 am	Workforce Development	Lois Curfman McInnes (PESO co-PI), Mary Ann Leung (Sustainable Horizons Institute)	Challenges and opportunities for broadening participation in the HPC workforce		
9:15 am	Breakout session				
10:15 am	Break				
10:45 am	Breakouts resume				
12:00 pm	Working Lunch				
12:30 pm	Report out from breakouts, discussion				
2:00 pm	Adjourn		4		

#### **PESO Vision**

# 100X

#### ECP investments enabled a 100X improvement in capabilities for target apps/libs

- 7 years building an accelerated, cloud-ready software ecosystem
- Positioned to utilize low-cost accelerators from multiple vendors that others cannot
- Emphasized software quality: testing, documentation, design, and more
- Prioritized community engagement: Webinars, BOFs, tutorials, and more
- DOE portability layers are the only credible way to
  - build codes that are sustainable across multiple GPUs and
  - avoid vendor lock-in or
  - deal with growing divergence and hand tuning in your code base
- DOE libraries and tools can lower costs and increase performance for accelerated platforms
- Industry has not caught up outside of Al
  - DOE enables an entirely different class of applications and capabilities to use accelerated nodes
  - In addition to AI

#### 100X\* your impact: Leveraging DOE/ECP investments

- Many communities still largely using home-grown solutions with room to improve. Opportunities:
  - Migrate from CPU to GPU For scale out to larger problems, or scale in to smaller GPU-enable systems (e.g., laptop)
  - Introduce modern software tools, workflows leverage the outreach, training and culture focused on improvement
  - Integrate into larger software communities E4S, xSDK, other software product communities
- How can we engage with these communities to realize the 100X improvement in science impact?
- DOE/ECP provides libraries, tools, expertise, and community connections that can be leveraged to realize 100X
- What are the best opportunities?
- What are the impediments?
- Can we produce strategic and tactical plans?
- Selling libraries and tools directly is hard to do ...
- Selling 100X impact across DOE, other agencies and industry could be much easier

\*100X (verb): to increase (your scientific impact) by two orders of magnitude

#### 100X Recipe

#### Ingredients

- A compelling science impact story
- **\$\$ \$\$\$**
- Staff
- Computing resources, training
- The deliverables and experience from DOE/ECP
- Delivered via post-ECP organizations like PESO
- And more...

#### Steps

- Translate science story to strategy and plan leverage experience from ECP, others
- ID node-level parallelization strategy CUDA, HIP, DPC++, Kokkos, RAJA, OpenMP, others
- Survey existing libraries and tools Vendors, E4S, others
- Explore available platforms DOE Facilities, cloud, others
- Leverage existing software ecosystem containers, Spack, others
- Leverage software communities Product communities, communities of practice, others
- Construct new codes within the broader ecosystem
- Produce new science results

#### More than one way to leverage 100X

- 100X can be realized as exciting new science capabilities at the high end
  - Fundamental new science on leadership platform
  - New opportunities for industry on affordable machines that fit in their data centers
- But it can also be used to reduce costs by running the same problems 100X cheaper
- Migration to accelerated platforms can be used to
  - Migrate a problem from an HPC cluster to a deskside or laptop systems
  - Lower your AWS monthly charges
  - Keep energy costs in check while still growing computing capabilities

#### Why are we here?

- To make 100X real
- To bring the people, communities, libraries, tools, methodologies from ECP into the future
- Many communities are here:
  - Application teams, Facilities, lab management, industry partners, US agencies, stakeholders
  - Library and tool developers, software community leaders
  - All: People who care about the impact of software on science
- To expand the community of engagement to include people who were not part of ECP we need you
- To organize the DOE scientific software community for optimal impact after ECP and beyond
- Outcomes:
  - Better understanding of the challenges, opportunities, and paths to success by everyone
  - Understand of next steps to pursue after leaving the workshop by everyone
  - To create a workshop report that furthers our strategic and tactical plans for success
  - Ultimately:
    - What do we gain financially by establishing a sustainability effort: Goal is success that brings funding
    - What do we lose in terms of management oversight: Goal is only the things that better and more easily done in aggregate



## PESO Project Description

Progress on defining PESO

Note: PESO is a work in progress!

Your contributions are essential to define and shape it!



#### PESO != ECP

#### ECP

- Hierarchy
- Centralized finance org
- Fixed set of apps, scope
- Heavyweight reporting
- Justified by size and design

#### PESO

- Peer collaboration Hub
- Leverage institutional finance orgs
- Dynamic, adaptive scope targets
- Tunable reporting strategy
- Lighter weight approach



### PESO > Spack+E4S

- Spack+E4S
  - Major PESO deliverable
  - Important product delivery conduits
  - Platforms for agency, industry collaboration
  - Keys for testing on new and diverse platforms & software environments

- PESO = Spack+E4S+More:
  - Impact on science via 100X efforts
  - Collaborative planning, executing tracking and reporting
  - HPC community engagement: apps, facilities, vendors, agencies
  - Cross-cutting training, community engagement, sustainability efforts
  - More

## PESO Project Brief Description



#### **PESO** will

- Serve as a hub for software-ecosystem sustainment efforts for DOE's open-source libraries and tools for advanced scientific computing
- Work with software project teams to coordinate development activities for long-term sustainability and benefit to stakeholders
- Work with
  - software product communities (SPCs) and
  - communities of practice (COPs)
- To provide cross-cutting services and support that are broadly needed by developers, users, and stakeholders
- Realize the full potential of DOE investments in the scientific libraries and tools ecosystem:
  - By taking a broad, strategic view
  - Through project growth, improved software quality and availability, and sustainable delivery, deployment, and support.
  - Realizing the 100X potential enabled by ECP investments

## PESO Sustainability Definition



- Sustained resources funding, effort, and infrastructure
- Robust user and developer base
- Focus: HPC libraries and tools ecosystem sustainability
  - Includes DOE, ECP, Advanced Scientific Computing scope as relevant
  - Critical functionality is sustained even as specific products come and go
  - Transitions into, out of, and within ecosystem are explicitly managed
  - Vendor products are integral to planning and collaborations
  - Evolution to meet community needs
- Critical mass:
  - Using hub and spoke approach to combine efforts
  - Leverage our aggregate scale for external influence

Briefly: What you do because you (want to) have users



## PESO Key Services and Activities

- Steer funding to key projects to maintain a robust software ecosystem in the long term
- Delivery and deployment via Spack and E4S to DOE Facilities, on-premise and cloud users and developers, including CI testing, issues triage, build caches, and software quality assurance
- Coordination of cross-cutting engagement with DOE Facilities, DOE sponsors, and other stakeholders such as other US agencies, US industry, and international partners
- Lightweight processes, models and tools to support software product communities with their software lifecycle management activities, including annual planning, execution, tracking, and assessment with change management
- Basic infrastructure for community engagement in coordination with communities of practice for outreach, training, community development, and coordination with external collaborators
- Outreach and workforce development to incubate new projects and grow the contributor base and external investment in key projects



#### **PESO Financial Model**

- Clear values and transparency: Product and community funding is based on a transparent set of criteria applied through an open review and assessment process
- Low overhead: Funds for all efforts at a particular lab are sent directly from the sponsor as a lump sum to the lab with itemized amounts for individual projects at that lab. Funds meant for university and industry subcontracts are sent from sponsor to the most appropriate partner lab. All funds at each lab are managed by the normal lab funding infrastructure



#### PESO PIER Plan

- Multifaceted approach to advance diversity, equity and inclusion throughout all work in the project, with emphasis on two complementary layers of scope:
  - Activities within the project and
  - Partnerships with others to plan and lead work toward culture change in our community overall
- In both contexts, we will address:
  - **Recruitment and inclusion**, with emphasis on engaging diverse individuals from underrepresented groups as members of our teams and community
  - Cultivating work environments that promote mutual respect and professionalism, with emphasis on sharing best practices and effecting culture change
  - Planning for scholarly and **professional growth of community members**, with particular emphasis on research software engineers (RSEs) and early-career staff



## Ways to participate in PESO efforts

- Invitation to engage in community planning: We invite community engagement through three complementary means
- Provide input via the <u>PESO Planning Input Google Form</u>
- We ask you to provide your input by May 25 for inclusion in the June 8
   9 workshop
- Engage in PESO Community Discussions (<a href="https://lssw.io/PESO">https://lssw.io/PESO</a>)
- Attend the PESO Community Workshop (<a href="https://bit.ly/peso-workshop-june2023">https://bit.ly/peso-workshop-june2023</a>)
- Attend PESO planning panel (virtual), June 20. Watch for announcment

### **Upcoming Events**



- PESO workshop: June 8 9, <a href="https://bit.ly/peso-workshop-june2023">https://bit.ly/peso-workshop-june2023</a>
- LSSW Meeting 13: 3 4:30 pm, June 15, Update on seed projects
  - https://lssw.io/Meeting13
- PESO Meeting 1: 3 4:30 pm ET, June 20, PESO Overview, Panel, Q&A
  - https://lssw.io/PESOMeeting1



# Seed project interactions



## Six seed projects

- COLABS: Collaboration for Better Software (for Science)
  - Lead Anshu Dubey, research software engineer (RSE) resources
- PESO: Toward a Post-ECP Software-Sustainability Organization
  - Lead Mike Heroux, cross-cutting hub to assist product lifecycle across aggregate ecosystem
- STEP: Sustainable Tools Ecosystem Project
  - Lead Terry Jones, performance tools ecosystem including DOE, non-DOE products
- SWAS: Center for Sustaining Workflows and Application Services
  - Lead Rafael Ferreira da Silva, workflows and app services ecosystem
- S4PST: Sustainability for Node Level Programming Systems and Tools
  - Lead Keita Teranishi, node-level programming ecosystem
- OSSF: Open Scientific Software Foundation
  - Lead Greg Watson, explore the role of software foundations to address sustainability

## All-seed projects May 2023 collaborations



- May 2023 updates
  - LSSw.io (<a href="https://lssw.io">https://lssw.io</a>)
    - Pointer to seed project proposals and web pages <a href="https://lssw.io/SeedProjects">https://lssw.io/SeedProjects</a>
    - Meeting 12: (May 18) Promoting inclusive and equitable research <a href="https://lssw.io/Meeting12">https://lssw.io/Meeting12</a>
  - Bi-weekly all-PI meetings with all seed projects
  - Focused meetings and workshops
    - Pair-wise sync up and outbriefing: May 18 19
  - PESO has initiated collaboration plans with STEP, S4PST, and SWAS seed projects
  - Collaboration options with COLABS and OSSF are under discussion

### PESO Hub and Spoke Approach



- Software Product Communities (SPCs), (aka, SDKs, Spokes)
  - PESO intends to be a hub that aggregates with communities compose of like products
  - We anticipate SPCs will self-organize and have community-specific governance
  - We anticipate SPCs to include DOE-sponsored and commercial/community software
  - SPC value proposition includes Shared design space exploration, coordination, more
- Communities of Practice (COPs)
  - PESO anticipates engaging with community leaders in important cross-cutting efforts
  - Examples include:
    - Scientific software developers: (e.g., IDEAS, HPC Best Practices webinars)
    - Community outreach (e.g., Center for Scientific Collaboration and Community Engagement (CSCCE)
    - Software foundations (e.g., NumFOCUS, Linux Foundation)
    - Workforce development (e.g., US RSE, BSSw Fellows, and Sustainable Research Pathways)
- Funding: Transparent criteria and process, with block funding





3 product community-focused seedlings: SWAS, STEP, S4PST

- If funded, these orgs would aggregate well with PESO
- We also expect to collaborate with other SPCs:
  - Math Libraries xSDK
  - Other libraries and tools that are not part of SWAS, STEP, S4PST but high priority
  - Emerging areas: Al for Science
- Focus on how these seeds and PESO will align
  - What they would need from PESO beyond their communities
  - How PESO could engage with key communities through them
  - Expected that these seeds will include non-DOE funded products



## The Seedling Landscape – Communities of Practice

3 broader meta-organizations (Hubs): PESO, COLABS, OSSF

- If COLABS or OSSF funded, PESO would
  - coordinate with and
  - coexist *alongside* these other organizations
- Looking for synergies and potential mismatches
- Trying to understand how funding models fit together



# Highlights from PESO Request for Input Responses



## How to improve software sustainability

- **Testing and Quality Assurance:** There's a strong emphasis on enhancing the testing infrastructure, including unit testing, continuous integration (CI), and deployment testing. This also involves establishing testing environments similar to user environments and using diverse application sets for testing. Also mentioned is the creation of a comprehensive test suite and regular code refactoring. Formalization and automation of development practices and procedures are seen as crucial.
- Portability and Maintenance: Several responses highlighted the importance of
  making the software compatible with newer languages and architectures, as well as improving
  portability on future systems. This includes maintenance activities for tools such as repositories, issue
  tracking, and CI, as well as humans for code reviews, bug fixing, training, and documentation.
  Maintenance of the project on major systems for testing and support was also mentioned.
- **Documentation and Training:** This includes improving and developing user and developer documentation, online short courses for users, tutorials, and other training materials. Some suggested that a software sustainability organization could provide a venue for sharing and highlighting documentation and tutorial development.
- Community Engagement and User Support: Responses suggested expanding the developer community, using modern community communication tools, and organizing training and outreach events. Efforts should also be made to increase the software's visibility, encourage more registrations, and identify users' potential needs. A suggestion was made to foster collaborations through a software sustainability organization to smoothen the user experience.
- Integration and Interoperability: This involves improving modularity of
  various features, integrating the software into larger communities, and providing interfaces to other
  packages. Better architectural documentation and support for application developers were also
  considered important.

- **Funding and Support:** Dedicated funding for software maintenance, quality assurance, documentation development, porting, and testing was recommended. If sustainability organizations provide personnel, the preference is for the personnel to work with the project team.
- Forward Planning and Innovation: Respondents mentioned feasibility studies for emerging technology and software engineering practices, as well as the need to innovate to address potential roadblocks such as language sustainability. Early access to upcoming technologies was also viewed as important.
- Standards and Automation: Some respondents advocated for driving standards and automating more aspects of the developer workflow, like code formatting and updates.
- Development of Advanced Features: The need for more efficient implementations for advanced hardware support, more fine-grained power monitoring, and support for modern workflows consisting of AI, Big Data, and Data Science workloads were also pointed out.

PESO, Software Product Communities, and Communities of Practice can positively impact most of these

# What a software sustainability organization should do to be a successful steward of DOE software



- **Funding and Stability:** Ensure a steady level of funding to support and sustain software products over the long term. It will help in retaining the talented team members and attracting new ones to participate and contribute.
- **Visibility and Engagement:** Increase visibility of software products and carefully choose engagement levels to avoid overstretching resources. Facilitate interactions between different groups developing software and help developers connect with users to understand their needs. Reach out to application developers and users actively.
- **Sustainability and Long-term Planning:** Acknowledge the fear of products not being sustained in the HPC community. Address this by explicitly sustaining products and assuring users that products will be maintained in the long run.
- **User Support and Usability:** Strive for a balance between user support and technological advancement. Ensure software is robust, has repeatable build and install instructions, and provides a clear description of usage expectations. Prioritize excellent user support in developing research libraries or tools.
- Documentation and Best Practices: Enforce good documentation practices, CI/CD practices, and circulate best practices across software packages. Advocate for best practices and provide conventions or standards for a uniform experience for application developers.
- Innovation and Avoiding Monoculture: Encourage innovation and avoid a situation where only a single dominant package/product is supported in any given category. Promote open-source software and ensure flexibility.

- Adaptation to Technological Changes: Adapt the software to changes in operating systems and GPU vendor software stacks. Improve software reliability, scalability, and performance based on user needs.
- Outreach and Collaboration: Foster community development, facilitate outreach to grow user base beyond traditional DOE HPC users, and establish mechanisms for meaningful collaborations.
- Portability and Composability: Ensure portability on future systems (including emerging architectures and programming models/languages), ensure composability with third-party tools.
- Integrated Approach: The organization should encompass various libraries and tools in an integrated manner so that end users and system administrators can deploy the stack easier.
- **Future Orientation:** Have a clear vision of the scientific communities' needs in the next decade and invest in highly performant sustainable software ecosystems.
- **Education and Awareness:** Raise awareness of the need for dedicated support and guidelines for best practices. The organization could also drive sustainability and adoption at the university education level.
- Quality Assurance and Simplified Installation:
   Provide as much quality assurance as possible and maintain simplified installation methods.

# Some factors for selecting and assessing a **F** product as part of the portfolio - **developers**

- User Base & Community: Assess the current and potential user base, both within specific domains (like the Department of Energy DOE) and across wider scientific and industrial applications. In addition, consider the size of the developer community, the participation of the product developers in the software community, and the vibrancy of the community that maintains and develops the product.
- **Relevance & Importance:** Evaluate the product's relevance and importance to its users and to the organization's mission, such as its criticality to technology, level of usage in high-performance computing (HPC) communities, and its inclusion in significant initiatives like large DOE hardware procurement or Software Development Kits (SDK).
- **Software Quality & Maintainability:** Look at the quality of the product, its maturity, and best software development practices. This includes unit testing, continuous integration/continuous delivery (CI/CD) practices with high test coverage, code quality, clear documentation, a good build system, and responsive, active development. The design of the product should encourage sustainable development.
- **Usability & Scalability:** Ensure the product is easy to use and can scale well to large problems and machines. This includes considering installation procedures, user support mechanisms, and deployability.
- **Performance & Portability:** The product should exhibit superior performance and be portable on future systems, taking into account the overall performance, scalability, and programmability of the software.

- **Support & Sustainability Plan:** Consider the level of support for the product, such as superior customer support, a supporting ecosystem around the product, and a dependable developer community. Furthermore, there should be a sustainable plan in place for long-term sustainment.
- Innovation & Potential for Growth: Evaluate the potential for the product to fill an unmet need in the community and its potential for growth, especially in emerging areas. A quick adoption rate could indicate high future impact.
- Alignment with Existing Portfolio: The product should be assessed in context with the existing portfolio and its alignment with the mission of the organization's portfolio. It's crucial to avoid unnecessary overlap with other products.
- **Openness & Extendibility:** Open-source products with numerous contributors, adherence to standards, and a well-maintained development community are highly preferred. Moreover, the software should be extensible and maintainable.
- Uniqueness & Added Value: The product's unique capabilities, either in performance or functionality, should be assessed, as well as the added value it brings to the community.

Across all factors: Balance between supporting successful, mature products and nurturing innovative, emerging ones.



# Some factors for selecting and assessing a product as part of the portfolio - facilities

- **Interaction with Vendors:** The relationship and communication channels with the software's creators or suppliers.
- **Performance Portability:** The software should have the ability to efficiently operate across different hardware configurations or operating environments.
- **User and Project Demand:** The software should have a significant user demand or meet the requirements of major projects.
- **Broad and Strategic Impact:** The software should have a widespread influence, particularly on strategic objectives such as enabling portability or enhancing key investments.
- **Support and Sustainability Models:** The mechanisms for maintaining and updating the software, and its long-term viability.

- Utilization by the HPC Applications Community:
   The software's usage rate and acceptance within the high-performance computing (HPC) community.
- **Community Interest and Participation:** The software should generate interest from the user community, who should be actively involved in its maintenance and enhancement.
- User Base and Potential for Growth: The software should have a large user base or the potential for one, and it should be vital enough to generate organic growth.
- **Impact and Value Added:** The software's influence on its user community and the added value it brings.
- **Infrastructure:** The software should provide valuable infrastructure to support its user base and future growth.
- **Vision for the Future:** The software should be forward-looking in all aspects, anticipating and accommodating future needs and trends.





- **Licensing:** The library or tool must have acceptable license constraints and restrictions. It should be compatible with the project's or organization's licensing terms.
- **Functionality:** The tool or library should be able to fulfill specific needs and improve productivity.
- **Developer and Community Support:** The tool or library should have ongoing support from its developers, including regular updates and bug fixes. A robust user and developer community is also crucial for problem-solving and help.
- Maturity and Documentation: The tool or library should have reached a level of maturity, proven stability and should have comprehensive documentation to assist its users.
- **Compatibility and Portability:** The library or tool should support the programming languages used in the project and be portable across different platforms.
- **Quality:** The library or tool should have a high standard of development quality, including extensive testing and active maintenance on bug reports and pull requests.

- Ease of Use and Learning Curve: The tool or library should be easy to use, have a short learning curve, and be capable of integration with other tools and libraries.
- Active and Welcoming Development Team: The team behind the library or tool should value user feedback and provide a supportive environment for users.
- Performance: The library or tool should deliver high performance and low latency.
- **Sustainability:** There should be recent development activity and a long-term support model, indicating a high likelihood that development will continue.
- **Vendor Support:** For some users, particularly in High Performance Computing (HPC) environments, vendor support may be a significant factor.
- Part of a Larger Ecosystem: The tool or library should preferably be part of a larger, friendly user base, like StackOverflow or other forums, which can offer additional support and resources.



#### Barriers to adopting an open-source library or tool

- Long-Term Viability Concerns: There are reservations about the durability of open source solutions for industry issues. Open-source projects often depend on community support and development, and their sustainability can be uncertain. A dedicated software sustainability effort can alleviate these concerns by ensuring ongoing support, development, and maintenance of these projects.
- Adapting to Evolving Hardware: With rapidly changing hardware platforms, software obsolescence is a significant concern. Sustainable software initiatives can help address this issue by ensuring that software remains compatible and efficient with the latest hardware advancements.
- **Software Licensing Issues:** Some pointed out the need for "Apache or better" software licenses that permit free commercial use. This barrier suggests a need for clear and open-source friendly licensing, allowing companies to adopt software without concerns over legal ramifications or costs. Software sustainability efforts can help ensure that the licensing of software promotes its widespread use and longevity.



#### User Base Growth – How a sustainability org can help

- **Collaboration and Community Engagement:** The user base for these packages primarily grows through collaborations, leveraging existing communities, and word of mouth. Various stakeholders advocate for more active engagement with communities through training sessions, workshops, and conferences.
- **Trust and Support:** Trust in the longevity and support for a software package is a crucial factor in its adoption. Sustainability organizations can play a key role in endorsing a package, thereby fostering trust among prospective users.
- Focus on Quality and Functionality: The four pillars of successful software projects are performance, robustness, usability/portability, and documentation & user support. Improving these aspects can significantly increase the user base.
- **Sustainable Funding and Support:** Continuous funding and support are necessary for maintaining and improving these software packages. Sustainability organizations could help provide this support, allowing for the development of new features and ensuring the software remains up-to-date and relevant.
- **Promotion and Awareness:** The role of sustainability organizations in promoting software packages is emphasized. This can involve various activities, including creating consultant positions, promoting the software in widely distributed newsletters, and providing opportunities for package developers to participate in relevant events and publications.



#### How facilities staff can contribute to DOE open-source libraries and tools

- Support highly configurable and scalable test and validation platforms. This will ensure that the software packages are thoroughly tested and validated for optimum performance.
- Collaborate with code teams to work on porting the software. The focus would be on making the software portable and sustainable to support new hardware features and technologies. This would enhance the software's adaptability and longevity.
- Offer in-kind support for troubleshooting and improving the software packages. There's also a potential for paid support. This provides an avenue for technical assistance and continuous improvement of the software packages.



### Outreach Support – How a sustainability org can help

- **Organization and Support:** Assistance in organizing and supporting these activities is frequently requested. This includes support for staff and infrastructure, coordinating courses and workshops, and helping with technical aspects like containerization, integration through Jupyter notebooks, advertising, etc.
- **Endorsement and Advocacy:** Some organizations could benefit from official endorsements, or advocacy within specific networks and programs.
- **Expanding User Base:** A sustainability organization could help identify new groups that could benefit from these tools or assist in diversifying the user base by reaching out to communities like AI, Big Data, and Data Science.
- Increasing Visibility: There's a desire for sustainability organizations to help increase the visibility of these tools beyond current circles.
- **Development Support:** This could involve helping with the addition of functionalities, documentation, and improvement of build systems.



## Takeaways from Input Responses

- Strong community awareness of importance of sustainability
- Strong common requirements and strategies
- Conjecture: An organization like PESO can be defined to provide:
  - Better What we produce will be better than with PESO
  - Faster
     — We will get our work done more quickly
  - Cheaper We can focus our efforts on other important things

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5:00 pm	Adjourn		Dinner on your own	

## Agenda

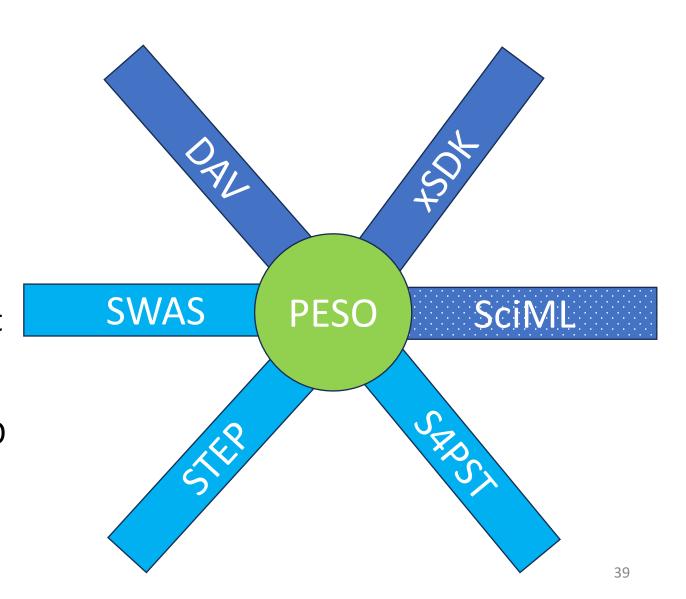


Friday, June 9, 2023				
Time (CT)	Topic	Leads	Comments	
7:30 am	Working Breakfast			
8:30 am	Challenges and Opportunities for Computing	Rick Stevens (ANL, Assoc Lab Director, Computing, Environment and Life Sciences)	Roles of sustainable software ecosystems in addressing next-generation computing challenges	
8:45 am	Software Foundations	Todd Gamblin (PESO co-PI)	How we can leverage software foundations for DOE software sustainability	
9:00 am	Workforce Development	Lois Curfman McInnes (PESO co-PI), Mary Ann Leung (Sustainable Horizons Institute)	Challenges and opportunities for broadening participation in the HPC workforce	
9:15 am	Breakout session			
10:15 am	Break			
10:45 am	Breakouts resume			
12:00 pm	Working Lunch			
12:30 pm	Report out from breakouts, discussion			
2:00 pm	Adjourn		38	

## PESO Hub-and-Spoke Status



- PESO (Hub) Funded seed for cross-community capabilities, engagements, services that are common to most or all software product communities
- **SWAS, STEP, S4PST** Funded seed projects for workflows, tools, programming systems
- DAV, xSDK Existing ECP SDKs that fit the PESO approach
- SciML Unmanaged product community that would fit the PESO approach
- Others Some products are missing – need to ID





## Hub and Spoke Status

- PESO SWAS, STEP, S4PST
  - Collaborating and evolving coordination within the hub-and-spoke model
- PESO xSDK, DAV
  - Working closely under ECP already
  - Includes ECP ST and Co-Design portfolios
- PESO SciML
  - Initial discussions to propose spoke for the scientific ML product stack
- PESO Other products
  - What is missing that should be included?