PESO: Partnering for Scientific-Software Ecosystem Opportunities

https://pesoproject.org

Lois Curfman McInnes, Michael Heroux, and the PESO team

DOE ASCR Computer Science PI Meeting
July 22, 2026

U.S. DEPARTMENT OF ENERGY · Argonne NATIONAL LABORATORY · BERKELEY LAB · Brookhaven National Laboratory · kitware · Lawrence Livermore National Laboratory · Los Alamos NATIONAL LABORATORY · OAK RIDGE National Laboratory · Pacific Northwest NATIONAL LABORATORY · ParaTools · Sandia National Laboratories · Team Libra · UNIVERSITY OF OREGON

PESO

Partnering for Scientific Software Ecosystem Stewardship Opportunities

https://pesoproject.org

The PESO Project exists to preserve, sustain, and advance the investments made by the Exascale Computing Project in a robust, versatile, and portable HPC software ecosystem and the people who make the ecosystem effective. Partnership with CASS.

PIs: M. Heroux and L.C. McInnes

PESO PARTNERSHIPS

STAKEHOLDER ENGAGEMENT AND CONSORTIUM PARTNERSHIPS

Consortium	Applications Community	Computing Facilities
Commercial HPC Companies	US Agencies	Industrial Users

COMMUNITY DEVELOPMENT

Better Scientific Software (BSSw) Fellowship Program

Workforce

KEY PESO GOALS

Enable applications to realize benefits of a software ecosystem
Emphasize software product quality, continued fostering of software product communities, and delivery of products, working with CASS

PESO SERVICES

INTEGRATION PARTNERSHIPS

Provide resources and support for portfolio build, integration, testing
- Spack integration
- CI testing
- Portfolio support & management

Collaboration with SSOs

SQA & SECURITY

Provide infrastructure to support and leverage product team SQA
- Supply chain, product quality
- Testing, documentation

PESO PRODUCTS

E4S AND SPACK

Support for product integration
Features for consortium products
Documentation, training

PORT & TEST PLATFORMS

Frank test & devpt system
Cloud resources
Documentation, training

BSSw.io CONTENT

Articles on scientific software productivity and sustainability

Scientific software ecosystem benefits (technical and community)

100,000+
Lines of code replaced with high-quality libraries and tools

10,000+
Community members via ecosystem collaborations

1,000+
Code teams share ecosystem costs and benefits

100+
Speedup using advanced devices like GPUs

10+
Reduction in build times via Spack build caches

1
Source code base for all computing systems

July 2026

Stakeholders:
Applications Community
Commercial HPC Companies
Industrial Users
US Agencies

Computing Facilities:
ALCF, NERSC, OLCF

CRLC:
ANL, BNL, LBNL, LLNL, LANL, ORNL, PNNL, SNL

Advisory Team:
Bhimji (NERSC), Biven (JLab), Diachin (LLNL), Ferreira da Silva (ORNL), Kothe (SNL), Messer (OLCF), Pakin (LANL), Riley (ALCF)

CASS Consortium
PESO, CORSA, FASTMath, LEADS, RAPIDS, STEP, S4PST

DOE Program Managers
ASCR: H. Finkel, D. Rabson, B. Brown, S. Hier-Majumder, R. Pino
NNSA: S. Hammond

PESO Organizational Chart

PIs: Mike Heroux (ParaTools) and Lois Curfman McInnes (ANL)

PESO PARTNERSHIPS

STAKEHOLDER ENGAGEMENT (Mike Heroux, ParaTools)
CONSORTIUM PARTNERSHIPS (Terry Turton, LANL)

Strategic engagement with consortium partners, applications, facilities, industry and agencies
(in collaboration with and co-funded by SSOs)

William Godoy, ORNL, On-node programming systems (w. S4PST)
Rajeev Thakur, ANL, Inter-node programming systems (w. S4PST)
Sameer Shende, Univ of Oregon, Tools (w. STEP)
Sherry Li, LBNL, Math libraries (w. FASTMath)
Berk Geveci, Vicente Bolea, Kitware, Data and viz (w. RAPIDS)
Hannah Cohoon, LBNL, UDX and Workflows
Mahantesh Halappanavar, Eral Mutlu, PNNL, EDA software

Unfunded partners: Strategic engagement with NNSA,communities of practice, applications, facilities, industry and agencies

Cody Balos, LLNL, NNSA software (funded by NNSA)
Partners at ALCF, NERSC, OLCF (funded by facilities)
Liaisons: Ann Almgren (FASTMath), Miro Stoyanov (LEADS)

COMMUNITY DEVELOPMENT
(Lois Curfman McInnes, ANL)

Better Scientific Software (BSSw) Fellowship Program
Elsa Gonsiorowski, LLNL, Coordinator
Adam Lavely, LBNL, Deputy Coordinator

Workforce
Mary Ann Leung, Sustainable Horizons Institute
Daniel Martin, LBNL
Suzanne Parete-Koon, ORNL, HPC Community Group lead

Communication
Mike Bernhardt, Team Libra

PESO SERVICES

INTEGRATION PARTNERSHIPS
(Jim Willenbring, SNL)

Software portfolio management and integration
(in collaboration with and co-funded by SSOs)

Jacob Bludau, ORNL, On-node sys (w. S4PST)
Hui Zhou, ANL, Inter-node prog sys (w. S4PST)
Bill Hoffman, Tim Haines, Kitware, Tools (w. STEP)
Satish Balay, ANL, Math (w. FASTMath)
Patrick O'Leary, Kitware, Data & viz (w. RAPIDS)
Mikhail Titov, BNL, Workflows
Jeff Sharpe, SNL, NNSA software ($ by NNSA)

SQA & SECURITY
(David Bernholdt, ORNL)

Ross Bartlett, SNL; Berk Geveci, Kitware; Jim Willenbring, SNL; Damien Lebrun-Grandie, LANL, and integration/strategy teams

PESO PRODUCTS

E4S (Sameer Shende, U Oregon)

Luke Peyralans, Wyatt Spear, Jordi Alcaraz, Erik Keever

Spack (Todd Gamblin, LLNL)

Caetano Melone, Greg Becker (LLNL); Galbreath, Krattiger, Nesbitt (Kitware)

PORT & TEST PLATFORMS (T. Gamblin and S. Shende)

Partnership with U Oregon, cloud, etc.

BSSw.io CONTENT

Rinku Gupta, ANL; Ross Bartlett, SNL; Keith Beattie, LBNL; Pat Grubel, LANL; Mark Miller, LLNL; David Bernholdt, ORNL; Lois McInnes, ANL; Mike Heroux, ParaTools

Strategy & Integration – Members are part of other SSO teams & NNSA, for tight collaboration

Spack v1.2.0

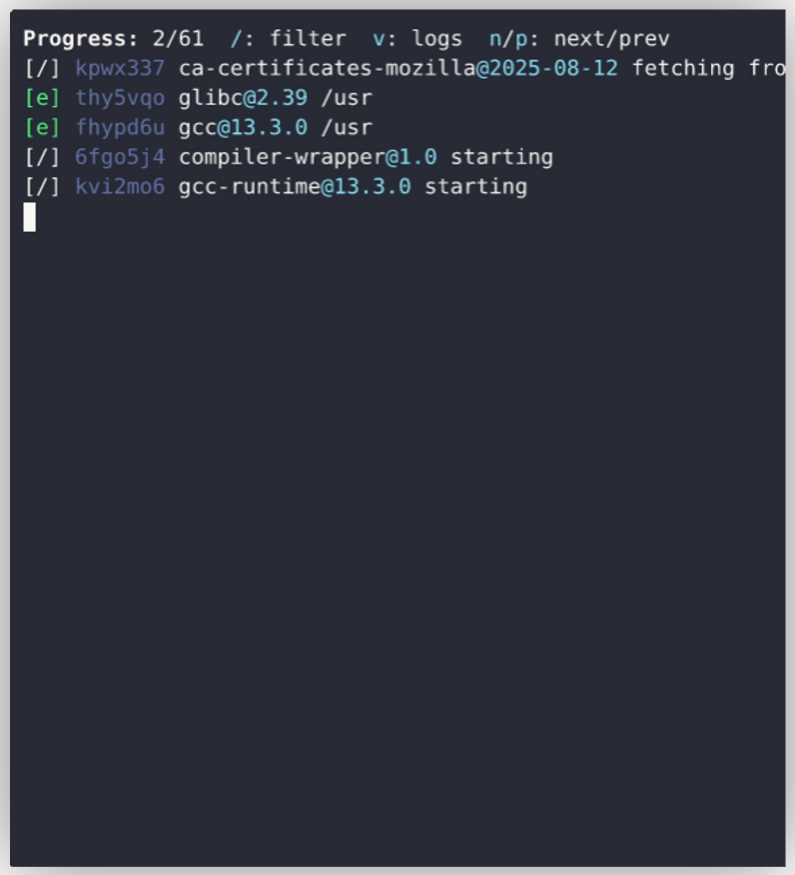
June 2026 release adds performance improvements and security features

Performance

- Parallel installer improves build performance by 2x or more
- Concretization caching speeds up repeated dependency solves by 2x+

Supply chain security

- Every build now includes a Software Bill of Materials (SBOM), allows scanning for CVEs
- Experimental build sandboxing with landlock (in Linux v5.13 kernel) ensures reproducibility, auditability, build environment safety



New parallel installer builds packages concurrently, allows work stealing

The AI ecosystem in Spack continues to grow

Spack contributors ensure latest AI builds are available for HPC

AI Packages

Hugging Face
py-transformers

JAX
py-jax
py-jaxlib

Scikit-Learn
py-scikit-learn

TensorBoard
py-tensorboard
py-tensorboardx

TensorFlow
py-tensorflow
py-tensorflow-datasets
py-tensorflow-metadata
py-tensorflow-probability

XGBoost
py-xgboost

PyTorch
py-botorch
py-gpytorch
py-kornia
py-lightning
py-pytorch-lightning
py-segmentation-models-pytorch
py-timm
py-torch
py-torch-geometric
py-torch-nvidia-apex
py-torchaudio
py-torchgeo
py-torchmetrics
py-torchvision
py-vector-quantize-pytorch

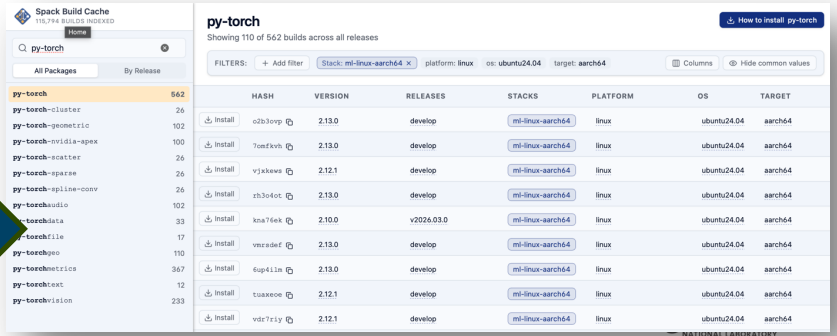
Platforms

macOS
aarch64

Linux
x86_64 / CPU
x86_64 / CUDA
x86_64 / ROCm

aarch64 / CPU
aarch64 / CUDA

Visit cache.spack.io for a searchable catalog



E4S provides a robust & growing software ecosystem for science

Open-source, portable, GPU-enabled libraries and tools (mod/sim, AI, and future QC)

https://e4s.io https://spack.io

- **E4S**: HPC-AI software ecosystem – a curated portfolio
- A **Spack-based** distribution of software tested for interoperability and portability to multiple architectures
- Available from **source, cloud, binary caches, containers**
- Not a commercial product – an open resource for all
- Regular releases, growing functionality: June 2026 E4S 26.06 – **125+ products**
- **One of the most important legacies of ECP**

Community policies
Commitment to SW quality

Curated collection
The end of dependency hell

Turnkey stack
A new user experience

DocPortal
Single portal to all E4S product info

Build caches
10X build time improvement

Portfolio testing
Especially leadership platforms

Post-ECP strategy (PESO & CASS)
Used across all computing facilities
work with vendors, advancing interoperability

Growing HPC-AI infrastructure for science

- NVIDIA Blackwell GPU CUDA v12.8 support
- NVIDIA NeMo™ and BioNeMo™ Frameworks
- Vllm inference engine
- Hugging Face Hub/CLI tools "GitHub of ML"
- TensorFlow, PyTorch, Horovod, JAX, sklearn, Pandas, Lbann, OpenCV, Torchbraid – GPU-optimized
- NVIDIA, AMD, Intel GPUs – portability
- Foundation for Adaptive Computing *Heidi AI*

Release presentation: https://e4s.io/talks/E4S_26.06.pdf

U.S. DEPARTMENT OF ENERGY Argonne National Laboratory is a U.S. Department of Energy laboratory managed by UChicago Argonne, LLC.

Leveraging and Supporting AI in E4S

E4S website AI features support users, E4S containers support AI research

E4S Guidebot, Prompt tables

- Guidebot:
  - Document-RAG GPT
  - Trained with Gemini deep reports
  - Served as custom OpenAI GPT
- Prompt tables:
  - Sets of attributes and definitions
  - Supports users in building effective prompts

E4S use of AI enhances discovery and usability of all ASCR apps, libs, tools

E4S base containers

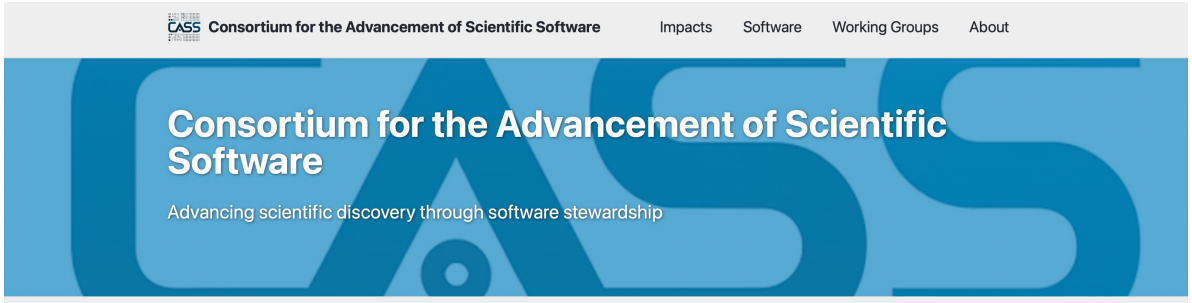
- Curated containers for CPUs/GPUs
  - Spack + pointer to binary caches
  - Container download < 1 min
  - Spack install/load of product ~ 1 min
- Example (Mac Laptop)
  - Docker pull on laptop: 42 sec
  - Spack install of LAMMPS: 75 sec
  - Parallel LAMMPS in 2 mins

E4S containers support reproducible, rapid access needed for AI workflows

Consortium for the Advancement of Scientific Software

Chair: D. Bernholdt
Vice Chair: J. Willenbring
Secretary: E. Raybourn

https://cass.community



Current CASS Members

SciDAC Institutes	Other Software Areas	Ecosystem and Crosscutting
FASTMath Scalable mathematical libraries	**S4PST** Programming models and runtimes	**PESO** Fostering, curating, and delivering a scientific software ecosystem
RAPIDS Platform readiness, data management / understanding, and AI tools	**STEP** Performance and correctness tools	**CORSA** Pathways to foundations, sw sustainability metrics
LEADS Scalable, customized scientific machine learning		

Current members are supported by DOE/ASCR Next-Generation Scientific Software Technologies (NGSST) and SciDAC programs

We are open to new members from DOE or elsewhere

What is CASS?

A **federation of member organizations** supporting specific communities or providing crosscutting capabilities related to **scientific software stewardship**

- CASS is a vehicle to **coordinate and collaborate** on activities that benefit the scientific software community, including developers, users, and other stakeholders

Software Catalog

Areas

Number of products in parentheses

Data and visualization (10)

Provide capabilities for analyzing, visualizing, compressing, moving, and managing data

Development tools (6)

Help address performance challenges and faciliate efficient support of the latest HPC node architectures

Mathematical libraries (14)

Scalable libraries supporting the latest HPC architectures for coupled systems, ensemble calculations, and more

Programming models and runtimes (11)

Support intra-node and inter-node concurrency on current and next-generation HPC node architectures

Software ecosystem and delivery (2)

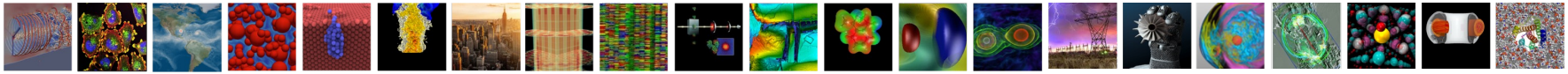
Provide software build, test, and integration tools, and containers environments

AND MORE …

Scientific Software Ecosystem Impact

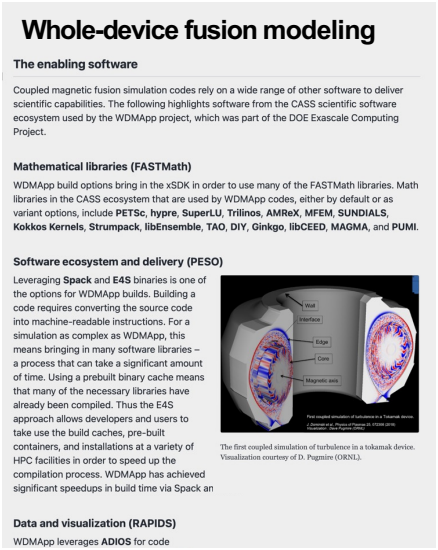
Basic science research in math/CS … enabling scientific discovery

https://cass.community



Thank you to Andrew Siegel, Erik Draeger, and ECP applications teams

Exemplar: WDMApp: Whole-device fusion modeling



Whole-device fusion modeling

The enabling software

Coupled magnetic fusion simulation codes rely on a wide range of other software to deliver scientific capabilities. The following highlights software from the CASS scientific software ecosystem used by the WDMApp project, which was part of the DOE Exascale Computing Project.

Mathematical libraries (FASTMath)

WDMApp build options bring in the xSDK in order to use many of the FASTMath libraries. Math libraries in the CASS ecosystem that are used by WDMApp codes, either by default or as variant options, include **PETSc**, **hypre**, **SuperLU**, **Trilinos**, **AMReX**, **MFEM**, **SUNDIALS**, **Kokkos Kernels**, **Strumpack**, **libEnsemble**, **TAO**, **DIY**, **Ginkgo**, **libCEED**, **MAGMA**, and **PUMI**.

Software ecosystem and delivery (PESO)

Leveraging **Spack** and **E4S** binaries is one of the options for WDMApp builds. Building a code requires converting the source code into machine-readable instructions. For a simulation as complex as WDMApp, this means bringing in many software libraries – a process that can take a significant amount of time. Using a prebuilt binary cache means that many of the necessary libraries have already been compiled. Thus the E4S approach allows developers and users to take use the build caches, pre-built containers, and installations at a variety of HPC facilities in order to speed up the compilation process. WDMApp has achieved significant speedups in build time via Spack an

The first coupled simulation of turbulence in a tokamak device. Visualization courtesy of D. Pugmire (ORNL).

Data and visualization (RAPIDS)

WDMApp leverages **ADIOS** for code

- **Software ecosystem and delivery (PESO):** Spack and E4S
- **Math libraries (FASTMath):** PETSc/TAO, hypre, SuperLU, Trilinos, AMReX, MFEM, SUNDIALS, Kokkos Kernels, STRUMPACK, libEnsemble, Ginkgo, libCEED, and MAGMA
- **Data and visualization (RAPIDS):** ADIOS, HDF5, PnetCDF, zfp, VTK-m, DIY
- **Programming models and runtimes (S4PST):** MPICH, Open MPI
- **Development tools (STEP):** TAU, HPCToolkit, PAPI and Darshan

AND MORE …

More info: https://cass.community/impacts/2025-01-wdmapp.html
Thank you to Amitava Bhattacharjee, C.S. Chang and the WDMApp team

PESO Team Contributes to HPSF Growth & Impact

HPSF Launch

- **The High Performance Software Foundation (HPSF),** launched May 2024, supports use and sustainment of apps, libraries and tools for leadership scientific computing
- HPSF promotes and incentivizes improved software quality, availability, and use through better team practices, processes, testing, and access to resources and events
- HPSFCon25: Over 200 DOE leaders, key industry, agency, and international partners
- **PESO team efforts and resources have been integral to HPSF growth and success**

HPSF
HIGH PERFORMANCE SOFTWARE FOUNDATION

hpsf.io

HPSF Impact and Promise

- HPSF promises to be the critical community element that brings together all parties with common interests in high-quality, open-source, scientific software
- HPSF provides funding and collaboration that enable DOE, other US agencies, industry, and international groups to work together on common software interests
- **HPSF provides a key element for sustaining DOE investments in scientific software**

PESO Roles in HPSF

- PESO members play key HPSF leadership roles; 10 PESO members attended HPSFCon
- PESO-supported products Spack and E4S are HPSF member products
- PESO-supported software integration staffing and the ”Frank” system with the latest GPU nodes provides critical CI testing for HPSF products

New Directions in 2026

- First European community summit
- HPSFCon 2026 grew to:
  - 237 attendees
  - 11 co-located project meetings
- Onboarding major new projects:
  - Flux, Environment Modules done
  - In progress:
    Open MPI, MPICH, LAMMPS

PESO Team Member Roles in HPSF

- **Todd Gamblin**: HPSF founder, Governing Board (GB) Chair, lead HPSF Core Project Spack
- **Damien Lebrun-Grandie:** GB member, HPSF Technical Advisory Committee (TAC) chair
- **Bill Hoffman:** TAC; **Jim Willenbring:** TAC, E4S Technical Steering Committee (TSC); **Sameer Shende:** E4S Project Lead/TSC member; **Greg Becker:** Spack; **Tammy Dahlgren:** Spack; **Ryan Krattiger:** Spack, Binaries WG lead; **Satish Balay:** E4S; **Luke Peyralans:** E4S; **Wyatt Spear:** E4S; **Mike Heroux:** E4S TSC member, HPSF “Cheerleader”

Community Development

HPSF Growth & Impact

HPSF
HIGH PERFORMANCE SOFTWARE FOUNDATION

https://hpsf.io

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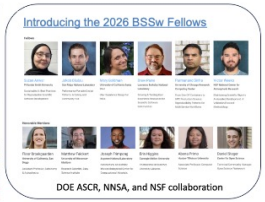
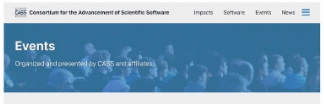
BSSw.io and BSSw Fellowship Program:

Fostering community and info on scientific software best practices



The Better Scientific Software Fellowship at US-RSE'25

HPC Best Practices Webinars … and more!



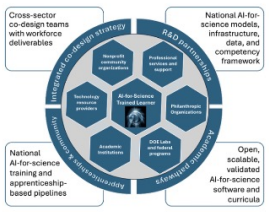
HPC Best Practices Webinars
The HPC Best Practices (HPC-BP) webinars address issues faced by developers of computational science and engineering (CSE) software on high-performance compu...

CASS BoF Days
CASS BoF Days provides opportunities to bring communities together for Birds-of-a-Feather (BoF) sessions around topics of interest.

Better Scientific Software Tutorials
The Better Scientific Software (BSSw) tutorials focus on issues of developer productivity, software sustainability, and reproducibility in scientific researc...

User/Developer Experience Webinars
User/Developer Experience Webinars feature speakers who highlight best practices and challenges for usable scientific software.

CASS Workforce Working Group



AI-for-science training and talent mobilization: Rapid-iteration model of co-design, co-development, and co-delivery

https://doi.org/10.6084/m9.figshare.31564060

Scientific Software Horizons Podcast

Scientific Software Horizons

Public group

Earn an Active Group badge

New podcast exploring what's next in scientific software and research computing … We're covering topics such as HPC, AI, and the evolving ecosystems that support modern scientific discovery.

- Join our Linked-In group
- Check out our YouTube channel

better scientific software
https://bssw.io/fellowship

PESO

Introducing the 2026 BSSw Fellows

Fellows

Suzan Anwar
Philander Smith University
Sustainable AI: Best Practices for Reproducible Scientific Software Development

Jakob Bludau
Oak Ridge National Laboratory
Performance-Portable Design Patterns: A Gallery and Community Hub

Mary Goldman
University of California Santa Cruz
User Experience Design for RSEs

Drew Paine
Lawrence Berkeley National Laboratory
Growing & Tending User Experience Resources for Scientific Software Communities

Parmanand Sinha
University of Chicago Research Computing Center
From One-Off Containers to HPC Production Science: Reproducibility Patterns for Multi-Service Workflows

Victor Weeks
NSF National Center for Atmospheric Research
Maintaining Scientific Rigor in AI-Assisted Development: A Validation-Focused Methodology

Honorable Mentions

Floor Broekgaarden
University of California, San Diego
Assistant Professor, Astronomy & Astrophysics

Matthew Feickert
University of Wisconsin-Madison
Research Scientist, Data Science Institute

Joseph Frimpong
Argonne National Laboratory
Postdoctoral Researcher, Midwest Integrated Center for Computational Materials

Erin Higgins
Carnegie Mellon University
Postdoctoral Researcher, University Libraries

Abena Primo
Huston-Tillotson University
Associate Professor, Computer Science

Daniel Steger
Center for Open Science
Technical Community Manager, Open Science Framework

DOE ASCR, NNSA, and NSF collaboration

The Better Scientific Software Fellowship at US-RSE'25

PESO Summary

Scientific software ecosystems: Working toward the future

- **ECP established the "Exascale Era"** showing the viability of Modeling/Simulation + AI computing systems for science
- **CASS and HPSF:** ECP's formal project approach has transitioned to:
  - A loose federal model (CASS: Consortium for the Advancement of Scientific Software, https://cass.community)
  - A foundation model (HPSF: High Performance Software Foundation, https://hpsf.io)
- **PESO's roles include:**
  - Stewarding and advancing E4S and Spack in open communities
  - Advancing the scientific software ecosystem
  - Supporting CASS by sponsoring leadership of crosscutting activities
- **Next frontier:** Software strategy for AI for Science: Integrating AI and Modeling/Simulation for impact
  - *Toward a Cohesive AI and Simulation Software Ecosystem for Scientific Innovation, 2024,* https://arxiv.org/abs/2411.09507

Explore more … posters

- PESO
- E4S: An HPC-AI Software Ecosystem for Science
- What's new in Spack 1.2
- User-Developer Experience (UDX)
- Advancing Software Practices and Impact: Sustainable DAV and TOOLS Integrations for DOE HPC software
- CASS: Software Stewardship for DOE/ASCR
- And also learn about S4PST, STEP, FASTMath, RAPIDS, LEADS