⬅️ Connect with CASS
https://tinyurl.com/2024-CASS-BOFS

CASS Community BOF Days

The Consortium for the Advancement of Scientific Software

June 11 – 13, 2024

https://cass.community/bofs

CASS Community BOFs 2024

https://cass.community/bofs

Date	Time (ET)	Topic (Select Title for Details)
June 11	11 am	Exploring the Landscape of AI and ML in Compiler Development: Pros and Cons
	11 am	Foundations Forum
	1 pm	Introducing CASS: The Consortium for the Advancement of Scientific Software
	3 pm	SUNDIALS User Experiences
	3 pm	Near-term Challenges and Opportunities for I/O

Date	Time (ET)	Topic (Select Title for Details)
June 12	11 am	MPICH: A High-Performance Open Source MPI Library for Leadership-class HPC Systems
	11 am	Differentiable and Portable Programming for Science
	1 pm	HPC Best Practices Webinar: Strengthening Development Workflows by Graphically Communicating Elements of Software Design - - Not a BOF but consider attending
	3 pm	ParaView and Catalyst
	3 pm	Building an Inclusive and Productive Community from Many Organizations to Support Software Stewardship
Date	**Time (ET)**	**Topic (Select Title for Details)**
June 13	11 am	Kokkos Ecosystem - State of the Union
	3 pm	Better Scientific Software Fellowship Community

Consortium for the Advancement of Scientific Software (CASS)

- **CASS Formation Team**
  - David Bernholdt
  - Phil Carns
  - Lois Curfman McInnes
- **Representatives of Software Stewardship Organizations (SSOs)**
  - **COLABS:** Anshu Dubey, David Bernholdt
  - **CORSA:** Greg Watson, Elaine Raybourn
  - **FASTMath:** Esmond Ng, Todd Munson
  - **PESO:** Mike Heroux, Todd Gamblin
  - **RAPIDS:** Rob Ross, Lenny Oliker
  - **S4PST:** Keita Teranishi, Damian Rouson
  - **STEP:** Terry Jones, Phil Carns
  - **SWAS:** Rafael Ferreira da Silva, Lavanya Ramakrishnan

BOF Plan

- Motivation
- Intro to CASS
- Intro to SSOs
- Discussion, Q&A

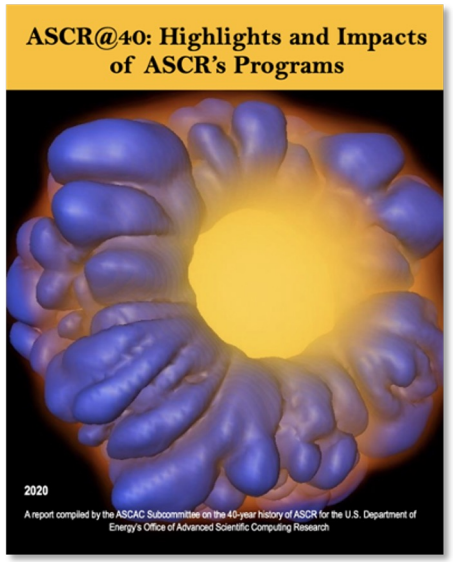
Reusable scientific software provides a foundation for discovery and innovation

ASCR: DOE's Office of Advanced Scientific Computing Research

***ASCR@40: Highlights and Impacts of ASCR's Programs*,** Hendrickson, Messina et al., 2020

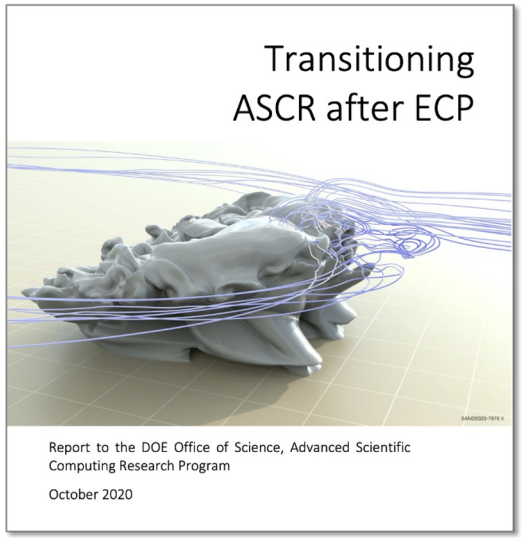
Challenges of the future

- Technology disruptions
- Funding balance
- **Software stewardship**
- Broader partnerships
- Sought-after workforce
- New roles for computing to advance science



***Transitioning ASCR After ECP*,** Giles et al., 2020

- **A. Advancing and Building on ECP**
- **B.** Advancing ASCR Research
- **C.** Current and Future Workforce



Challenge 3: Software Stewardship

The community has long struggled to settle on a good model for sustained support for key elements of the software ecosystem. This issue will get more acute as the Exascale Computing Project winds down and its large, focused software efforts are at risk of being left high and dry with no support for continued development or maintenance. **ASCR needs to recognize that software is really a scientific facility that requires sustained investments in maintenance and support. Improved and sustainable funding mechanisms are required.**

Closely related is the need for investments in improved software engineering practices reflecting profound changes in the way scientific software is developed and maintained. Modern scientific software is increasingly the product of large, dispersed teams and leverages a diverse suite of libraries and tools … Investments in developing, applying, and advancing best practices in software engineering for scientific applications will be essential for continued progress.

Recommendation A1: Create a shared-software stewardship program within ASCR

ASCR should create a comprehensive program that leverages the ECP ecosystem to support and curate shared software.

Stewardship is vital

Our community discussions indicated a strong consensus on the need for some form of software stewardship.

Leadership for the long term

We believe the software hub should be led by DOE laboratory and academic software leaders who possess long-term experience with DOE software development and delivery.

Exascale Computing Project

Maintain **international leadership in HPC**

Promote the **health of the US HPC industry**

Deliver a **sustainable software ecosystem** used and maintained for years to come

Ensure that exascale systems can be used to deliver **mission-critical applications**

ECP EXASCALE COMPUTING PROJECT

7-year, $1.8B

US Department of Energy project funded 1000+ people at national labs, universities, US industries

This research was supported by the Exascale Computing Project (17-SC-20-SC), a collaborative effort of the U.S. Department of Energy Office of Science and the National Nuclear Security Administration.

Application Development

- Develop and enhance the predictive capability of applications, **25 applications, 6 Co-Design Centers**

Software Technology

- Deliver expanded and vertically integrated software stack, **70 unique products**

Hardware and Integration

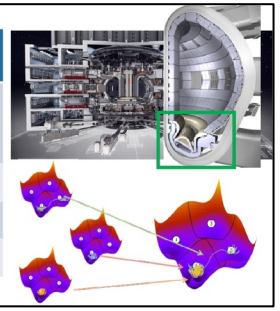
- Application integration and software deployment to facilities, exascale node and system design, **6 US HPC vendors**

NNSA National Nuclear Security Administration

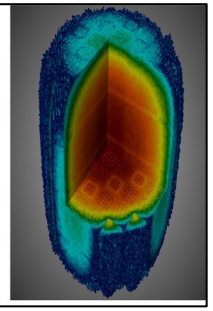
U.S. DEPARTMENT OF ENERGY | Office of Science

ECP software technologies power diverse applications across multiple architectures

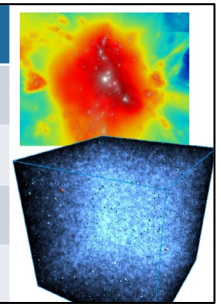
Project/PI	EXAALT: Molecular Dynamics Danny Perez
Challenge Problem	Damaged surface of Tungsten in conditions relevant to plasma facing materials in fusion reactors • 100,000 atoms • T=1200K
FOM Speedup	398.5
Nodes Used	7000
ST/CD Tools	Used in KPP Demo: **Kokkos, CoPa**



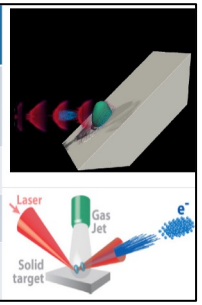
Project/PI	ExaSMR: Small Modular Reactors Steve Hamilton
Challenge Problem	NuScale-style Small Module Reactor (SMR) with depleted fuel and natural circulation • 213,860 Monte Carlo tally cells/6 reactions • 5.12×10^{12} particle histories/cycle, 40 cycles • 1098×10^{6} CFD spatial elements • 376×10^{9} CFD degrees of freedom • 1500 CFD timesteps
FOM Speedup	70
Nodes Used	6400
ST/CD Tools	Used in KPP Demo: **CEED** Additional: Trilinos



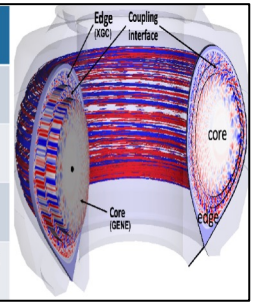
Project/PI	ExaSky: Cosmology Salman Habib
Challenge Problem	Two large cosmology simulations • gravity-only • hydrodynamics
FOM Speedup	271.65
Nodes Used	8192
ST/CD Tools	Used in KPP demo: **none** Additional: CoPa, VTK-m, CINEMA, HDF5.0



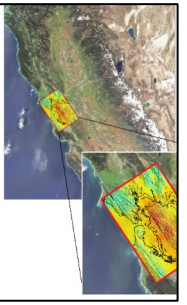
Project/PI	WarpX: Plasma Wakefield Accelerators Jean-Luc Vay
Challenge Problem	Wakefield plasma accelerator with a 1PW laser drive • 6.9×10^{12} grid cells • 14×10^{12} macroparticles • 1000 timesteps/1 stage
FOM Speedup	500
Nodes Used	8576
ST/CD Tools	Used in KPP Demo: **AMReX**, **libEnsemble** Additional: ADIOS, HDF5, VTK-m, ALPINE



Project/PI	WDMApp: Fusion Tokamaks Amitava Bhatacharjee
Challenge Problem	Gyrokinetic simulation of the full ITER plasma to predict the height and width of the edge pedestal
FOM Speedup	150
Nodes Used	6156
ST/CD Tools	Used in KPP Demo: **CODAR**, **CoPA**, **PETSc**, **ADIOS** Additional: VTK-m



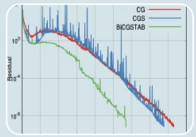
Project/PI	EQSIM: Earthquake Modeling and Risk Dave McCallen
Challenge Problem	Impacts of Mag 7 rupture on the Hayward Fault on the bay area.
FOM Speedup	3467
Nodes Used	5088
ST/CD Tools	Used in KPP Demo: **RAJA, HDF5**

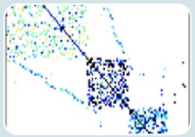


ECP Software Technologies

- Prepare SW stack for scalability with massive on-node parallelism
- Extend existing capabilities when possible, develop new when not
- Guide, and complement, and integrate with vendor efforts
- Develop and deliver high-quality and robust software products

70 software products across 6 technical areas





Programming Models & Runtimes
- Enhance and get

Development Tools
- Continued, multifaceted

Math Libraries
- Linear algebra, iterative linear solvers, direct linear solvers, integrators

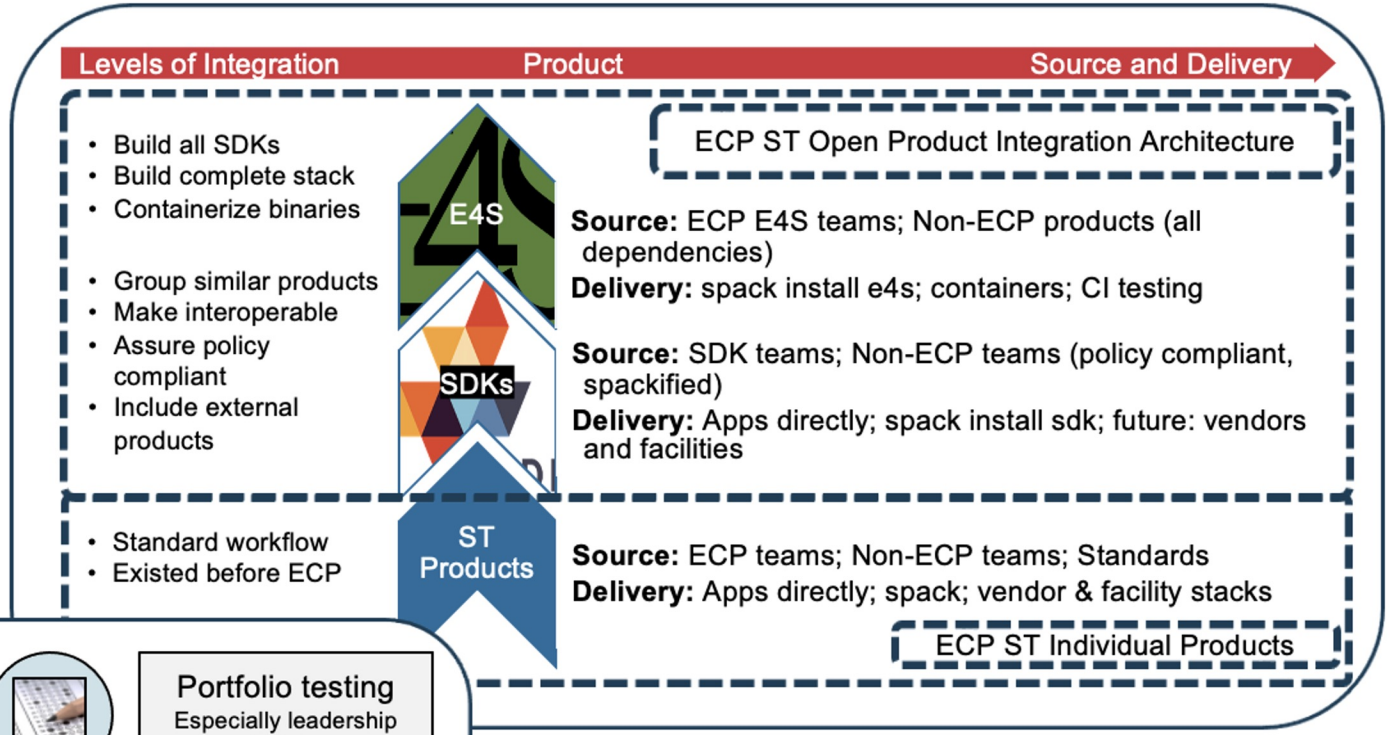
Data and Visualization
- I/O via the HDF5 API

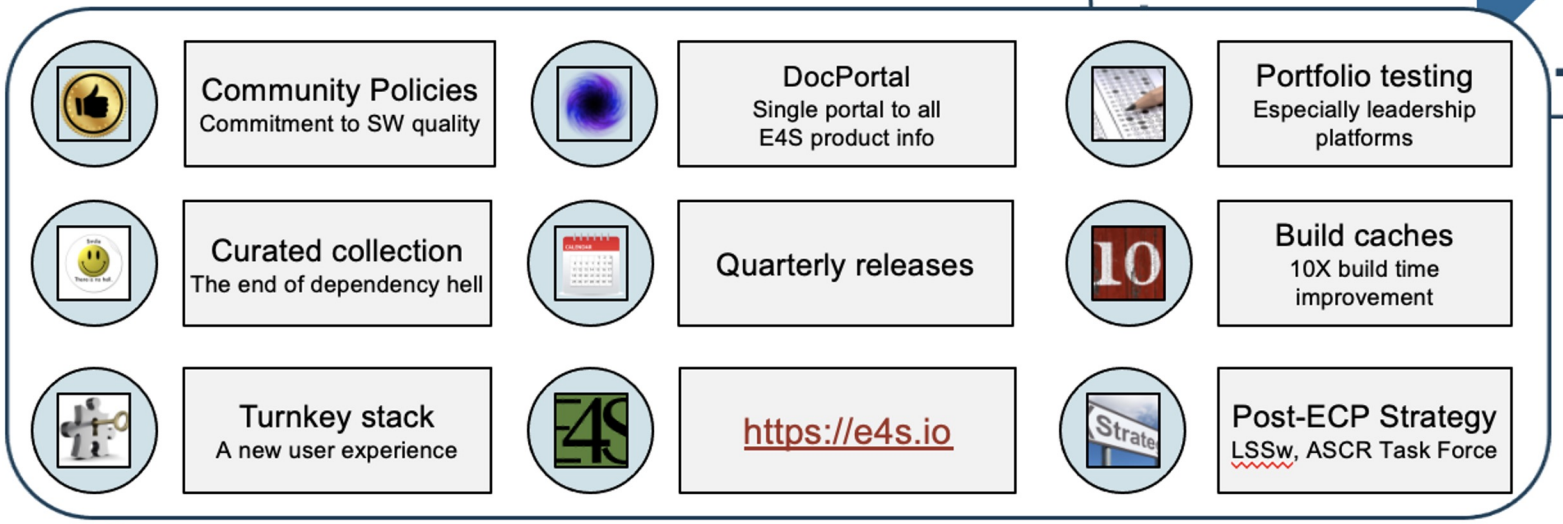
Software Ecosystem
- Develop features in Spack necessary to

NNSA ST
- Open source NNSA Software projects
- Projects that have

A robust HPC scientific software stack – for exascale and beyond

- ECP Software Technology lead: Mike Heroux (SNL)
- E4S: HPC software ecosystem – a curated software portfolio
- A **Spack-based** distribution of software tested for interoperability and portability to multiple architectures
- Available from **source**, **containers**, **cloud, binary caches**
- Not a commercial product – an open resource for all
- Supported by DOE and commercial entities (Paratools)
- Growing functionality: November 2023: E4S 23.11 – 100+ full release products





https://e4s.io

E4S lead: Sameer Shende (U Oregon)

Spack https://spack.io

Spack lead: Todd Gamblin (LLNL)

Announcing CASS

The Consortium for the Advancement of Scientific Software

CASS Basics

- A newly-formed organization
- Sponsored by DOE Office of Advanced Scientific Computing Research (ASCR)
- Established by DOE Software Stewardship Organizations (SSOs)

CASS Goals

- Forum for SSO collaboration and coordination
- Bigger than the sum of its parts
- Vehicle for advancing the scientific software ecosystem

CASS Status

- Defining governance structure
- Establishing community awareness
- Building a team of teams
- Collaborating on outreach

Software Stewardship Organization (SSO) Basics

- Each SSO represents a specific software ecosystem concern
- **Product SSOs:** Programming systems, performance tools, math packages, data/viz packages
- **Portfolio SSO:** Curating & delivering software stack to the community
- **Community SSOs:** Workforce, partnerships

Engage with CASS

- Participate in June 11-13 CASS Community BOF Days: https://cass.community/bofs
- Visit https://cass.community

8 Software Stewardship Organizations (SSOs)

DOE Office of Advanced Scientific Computing Research (ASCR) Post-ECP Projects

COLABS

Training, workforce development, and building the RSE community

CORSA

Partnering with foundations to provide sustainable pathways for scientific software

FASTMATH

Stewardship, advancement, and integration for math and ML/AI packages

PESO

Stewarding, evolving and integrating a cohesive ecosystem for DOE software

RAPIDS

Stewardship, advancement, and integration for data, visualization and ML/AI packages

S4PST

Stewardship, advancement and engagement for programming systems

STEP

Stewardship, advancement of software tools for understanding performance and behavior

SWAS

Stewardship and project support for scientific workflow software and its community

CASS Charter (Draft May 2024)

Also drafts of CASS by-laws and strategies for stakeholder engagement

Name

The name of the organization is the Consortium for the Advancement of Scientific Software (CASS) (the Consortium).

Mission

Stewardship and advancement of the current and future ecosystem of scientific computing software.

Principles

- **Transparency**: open governance policies and open access to Consortium artifacts.
- **Diversity**: cultivation of diverse participation and representation.
- **Sustainability**: long-term viability and growth of software, practices, and workforce.
- **Innovation**: responsiveness to stakeholder needs and technological evolution.
- **Cooperation**: working together to support the overall Consortium mission.
- **Integrity**: acting as a fair, trusted, and respected asset to the community.

Organizational Model

The Consortium is a federation of member organizations committed to actively pursuing the stated Mission and Goals in a collaborative fashion, following the stated Principles. Member organizations exist to support specific communities or to provide crosscutting capabilities related to scientific software stewardship. Member organizations coordinate and cooperate as a Consortium to maximize benefit to the ecosystem as a whole.[1]

Goals and Scope

In support of the mission and principles, in conjunction with its member organizations, the Consortium will:

- Deliver a capable, high-quality, interoperable software ecosystem for scientific computing –
  By providing guidance with respect to software engineering best practices and standards; developing, promulgating, and applying assessment methods.
- Build and retain a diverse, inclusive, and capable workforce equipped to carry out and lead scientific software stewardship and advancement activities –
  By fostering a supportive and inclusive culture and applying best practices to broaden participation.
- Engage a wide base of stakeholders –
  By promoting the scientific software ecosystem, undertaking outreach activities to educate and engage, lowering barriers to engagement, and pursuing opportunities to broaden the impact of the Consortium.
- Maintain open, two-way communication with stakeholders –
  By speaking with a unified voice to stakeholders regarding status and direction, and disseminating feedback to the Consortium.
- Maximize the impact of Consortium resources and capabilities for the benefit of the ecosystem at large –
  By improving efficiency by combining and coordinating infrastructure, planning, and resources across the ecosystem.
- Maintain situational awareness and balanced coverage of the evolving needs of scientific computing –
  By identifying gaps, incompatibilities, and other issues to be addressed in a coordinated fashion across the Consortium.
- Ensure the long term viability and sustainability of the Consortium –[2]
  By exploring and executing plans for ensuring secure funding sources, including growth of the Consortium through the expansion of membership.

Stakeholders

Stakeholders in the Consortium include the following scientific software ecosystem participants[3]: users, producers, computing facilities, funding organizations, vendors, industry, agencies, and institutional leaders. They are not restricted by national, commercial, or organizational boundaries.

Roles and Responsibilities

The Consortium-level governance consists of the entities defined below.

The **Steering Committee** is responsible for ensuring that the Consortium as a whole complies with the mission statement and charter. The Steering Committee includes representation from each constituent member organization.

The **External Advisory Committee** is responsible for providing guidance to the Steering Committee from an objective external perspective. It is composed of a diverse selection of stakeholders or other subject matter experts who are not themselves members of or directly supported by the Consortium.

Working Groups will be created as needed by the Steering Committee to carry out specific objectives of the Consortium. Working Groups may be composed of member organization participants or external parties. The objective, scope of activity, duration, and size of each Working Group will be clearly defined at its inception.

Member organizations define their own governance structure for topics that are outside the purview of the Consortium.

[1] A minor update is needed here to reflect the affiliate membership tier concept that has been added to the by-laws.

[2] This item is under active discussion if it is within scope and appropriate for the Consortium in its current form.

[3] Our intent is to synchronize this with the stakeholder engagement plan document; any discrepancy is unintentional.

COLABS: Collaboration for Better Software (for Science)

Motivations and Objectives

Helping software teams produce better software

- Training and complementary resources on software productivity and best practices
- Coordination of training development and delivery for CASS
- Advocacy for better software practices with sponsors, project leaders, and developers

Helping grow and enrich the workforce of software professionals

- Building the research software engineering (RSE) community of practice (CoP) in the national laboratories
- "Onboarding training" to support broader candidate pools for software professional positions
- Filling the pipeline: outreach to colleges for internships and careers

Training and Related Resources

An extensive training program for software productivity and best practices

- Building on the successful Better Scientific Software (BSSw) tutorial series, originated in the IDEAS project (> 30 events since 2016)
- Collaborating with related training efforts in the community

Providing related resources

- HPC Best Practices webinar series (monthly cadence)
- Better Scientific Software (BSSw.io) resource site (w/ PESO)

Coordination of training for CASS

Advocacy for better software practices

Building the DOE RSE CoP

Build interactions, knowledge sharing among RSEs at national labs

- Encouraging social interactions
- Sharing of technical and professional knowledge and experiences
- In collaboration with U.S. Research Software Engineer Association (US-RSE)

Other Workforce-Building Efforts

Onboarding training

- Expand applicant pools by developing training curricula to allow new hires to acquire needed skills
- Both technical and "soft" skills

Retention-enhancing practices for software projects

- Identify and promote practices software projects and organizations can implement to improve employee satisfaction and retention

Filling the pipeline

- Outreach to colleges (esp. MSIs) to promote internships and careers in research software engineering

Team

Argonne National Laboratory: Anshu Dubey (Lead PI), Rinku Gupta
Oak Ridge National Laboratory: David Bernholdt (PI), Greg Watson
Lawrence Berkeley National Laboratory: Dan Gunter (PI), Keith Beattie
ASCR PM: David Rabson

Note: Phase-2 proposal is pending

Argonne NATIONAL LABORATORY
OAK RIDGE National Laboratory
BERKELEY LAB

CORSA: Center for Open-Source Research Software Advancement

CORSA is a five-year post-ECP software-ecosystem stewardship and advancement project. In partnership with the Consortium for the Advancement of Scientific Software (CASS), CORSA will become a community of practice that creates pathways for open-source scientific software projects to avail themselves of resources for long-term growth, stewardship, advancement, and innovation.

Goals

Create pathways to open source software foundations

Empower communities with software sustainability metrics

Facilitate cross-cutting activities to address the needs of unique and diverse communities

Provide objective guidance to software communities

Activities

- **Foundation Forum**: We lead CASS efforts for enabling software projects to leverage open source software foundations as a pathway toward sustainability
- **Software Sustainability Metrics**: We will work with the community to develop software sustainability metrics and coordinate mechanisms to collect and utilize metrics to best serve the needs of CASS members
- **Best Practices**: We gather successful project and community experiences to create a repository of best practices, example documents, and guidance that can be used by software projects in their sustainability efforts
- **Guidance and Training Resources:** Curate and create guidance and training resources to share and disseminate strategies for sustainability activities

Pathways to Foundations for Scientific Software Projects

Scientific Achievement

CORSA is developing material to help software projects make decisions about joining software foundations, and then to actually join them. This initially includes guidance for joining NumFOCUS, and examples and guidance on work the project needs to do internally as part of this process.

Significance and Impact

Joining a software foundation can be part of a software project's path to sustainability, leading to potential increased visibility and funding via the foundation's partners and collaborators. A foundation is also a set of partner projects that can share experiences and lessons. CORSA is working to help projects understand multiple foundations, and how to join them via documents and sessions at community events

Technical Approach

- Working with NumFOCUS, we have developed https://corsa.center/foundations/numfocus.html to help projects understand the process of joining NumFOCUS and the potential benefits and costs. We will expand this to other foundations.
- We have also developed guidance, documents, examples, templates (https://github.com/corsa-center/oss-documents/) such as on governance, roadmaps, contributing, code of conduct, licenses, etc., which projects need to have in order to join a foundation.
- We will be reaching out to scientific open source projects from ECP and beyond via sessions, talks, and posters at events such as PASC, US-RSE, SC, eScience, SIAM CSE, …

NumFOCUS's fiscally-sponsored projects (as of April 2024), including many projects supported by DOE and/or essential to DOE science

PI: Gregory R. Watson, Oak Ridge National Laboratory
Collaborating Institutions: HDFG, Kitware, SNL, UIUC
ASCR Program: Software Stewardship and Advancement
ASCR PM: David Rabson
Resources: https://corsa.center; https://cass.community

Effective Metrics for Measuring and Enhancing Sustainability in Scientific Software

National Laboratories Information Technology Summit 2024 (NLIT'24)

Scientific Achievement

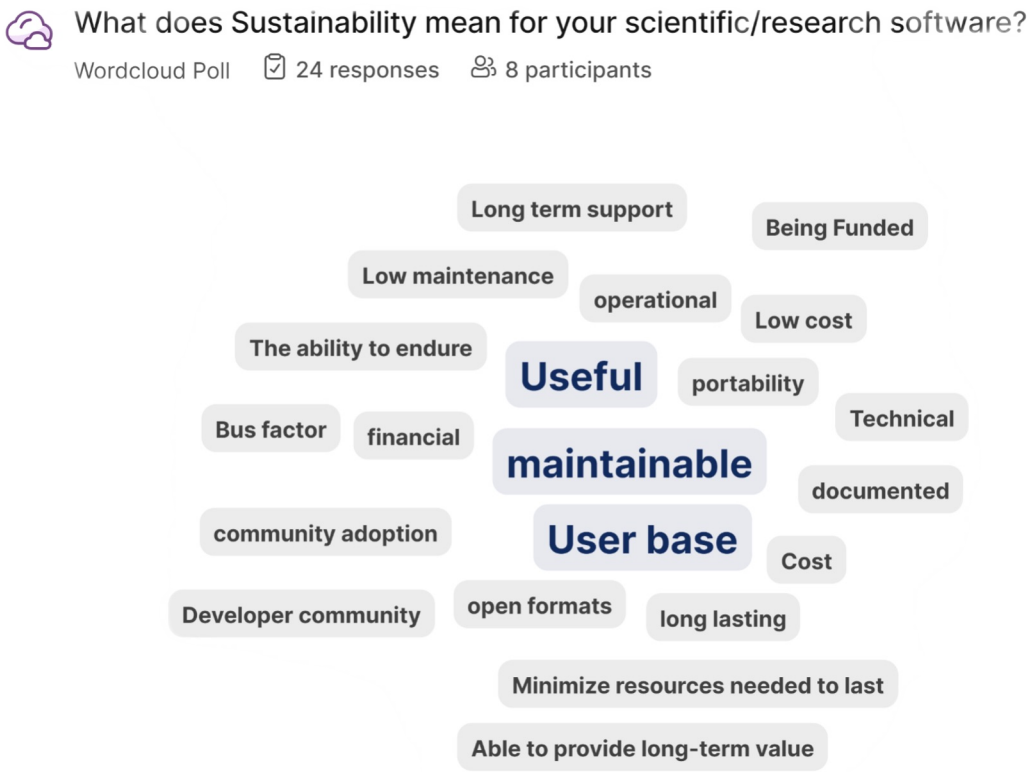
CORSA is working to help scientific software projects understand how metrics can be used to gain insights about their sustainability efforts. We held a first workshop to engage with representatives of PESO, STEP, and FastMATH at the NLIT'24 workshop.

Significance and Impact

Software and project metrics are the recognized method for measuring community health, software quality, and sustainability. However, little work has been undertaken to understand the specific needs of scientific software. This workshop is the first in a series of events to engage with this community to define and interpret metrics for measuring sustainability. We are also working with the Community Health Analytics in Open Source Software (CHAOSS) and Open Source Security Foundation (OpenSSF) to help define, collect, and interpret metrics.

Technical Approach

- Hold meetings and workshops with stakeholders to collect requirements
- Undertake surveys, literature reviews, and studies to assess effectiveness
- Provide infrastructure to enable the collection, interpretation, and dissemination of sustainability metrics



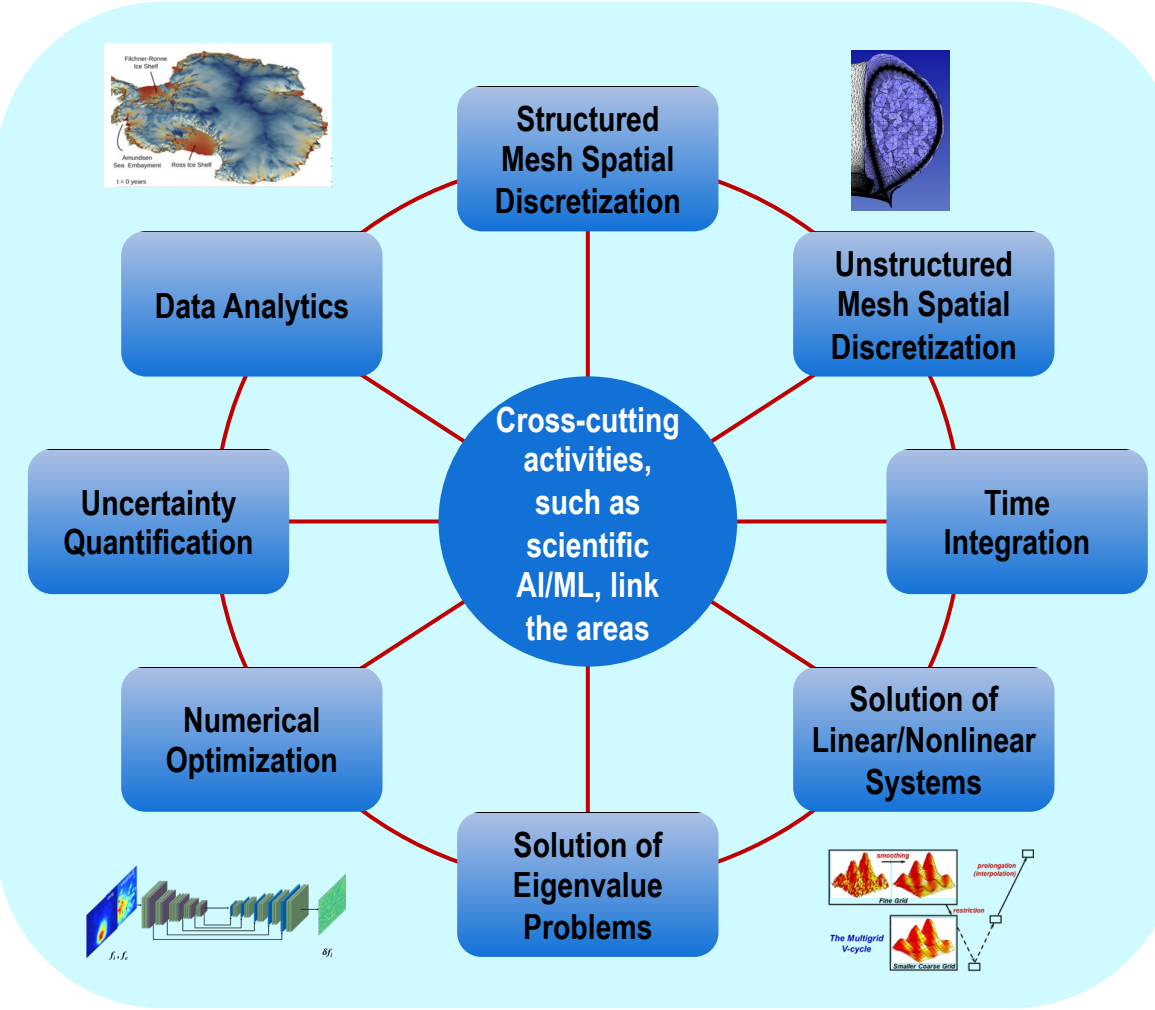
A poll from workshop interaction activity asking the workshop participants: What does sustainability mean for their scientific/research software. These provide an indication of the various aspects important to projects' sustainability.

PI: Gregory R. Watson, Oak Ridge National Laboratory
Collaborating Institutions: ANL, Berkeley, Kitware, HDFG, LLNL, LANL, UIUC
ASCR Program: Software Stewardship and Advancement
ASCR PM: David Rabson
Resources: https://corsa.center; https://cass.community

FASTMath – SciDAC Institute on Frameworks, Algorithms and Scalable Technologies for Mathematics

Provide leading edge applied and computational mathematics to remove the barriers facing computational scientists

- Develop robust math techniques and numerical algorithms for DOE science problems
- Deliver highly performant software with strong software engineering to run efficiently and scalably on DOE supercomputers
- Work closely with domain scientists to leverage our math and ML expertise and deploy our software in large-scale scientific codes
- Build and support the broader computational math and computational science communities across DOE

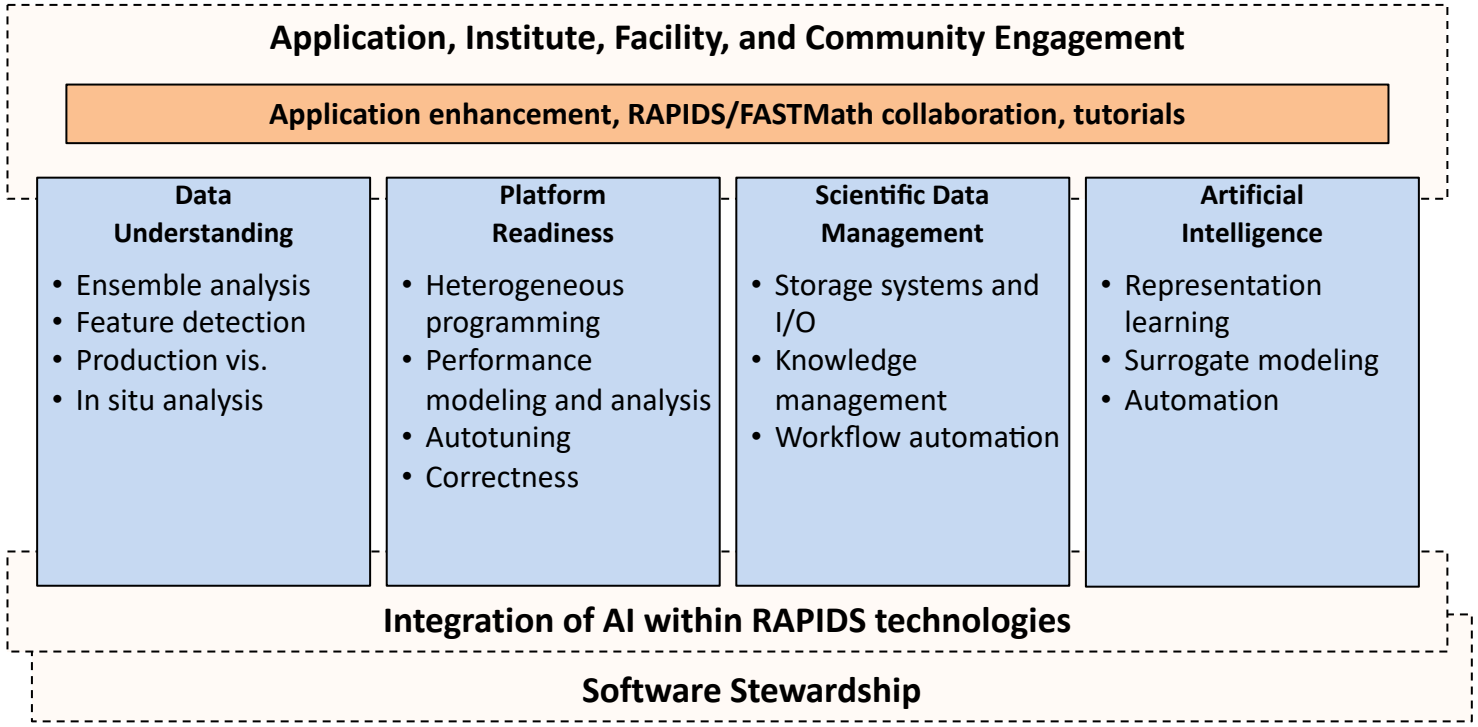


Director: Esmond G. Ng (LBNL)
Deputy: Todd Munson (ANL)

The SciDAC RAPIDS Institute

Enabling scientific breakthroughs using DOE supercomputers by assisting SciDAC and DOE scientists and engineers to solve computer science, data, and artificial intelligence (AI) challenges.

- **Four thrust areas covering key needs**
- **Emphasis on enabling AI/ML use by science teams and leveraging within RAPIDS tools**
- **Software stewardship activities targeting widely used software packages**



Software Stewardship in the RAPIDS and FASTMath Institutes

Objective

The objectives of stewardship activities within RAPIDS and FASTMath are to advance and steward a selected set of production software products for use in leadership computing providing key capabilities to DOE science teams, to help bring relevant new software products to a production state, and to foster the integration of software tools into effective solutions that help achieve DOE mission objectives.

Significance and Impact

A robust software ecosystem is a critical enabler of DOE science, helping adapt to the evolution of the underlying hardware technology ecosystem and evolving DOE mission needs.

Technical Approach

- Utilize stakeholder input to identify priority software products, working with other SSOs to identify key capability gaps and avoid duplication of effort
- Fund product-specific activities that improve the software in terms of impact, quality, and/or sustainability
- Leverage the wealth of knowledge in the ASCR and technical computing communities to identify promising potential products for “incubation”
- Actively collaborate with our peer SSOs to train software teams on best practice, to integrate into the broader software ecosystem, to gain access to CI/CD resources, and to build connections between teams
- Promote equity and inclusion as an intrinsic element to advancing scientific excellence

Name	Summary
Data	
ADIOS	ADIOS provides a simple, flexible way for scientists to describe the data in their code that may need to be written, read, or processed.
DIY	Block-parallel library for writing scalable parallel algorithms
HDF5	Parallel I/O library for high performance access to self-describing HDF5 datasets
Paraview/Catalyst	ParaView is a tool for post hoc visualization at scale. Catalyst is the associated in situ library.
PnetCDF	Parallel I/O library for high performance access to self-describing netCDF datasets
VisIt/Ascent	VisIt is an open source, interactive, scalable, visualization, animation and analysis tool. Ascent is a lightweight in situ library leveraging VTK-m for GPU support.
VTK-m	VTK-m is a performance portable visualization library leveraged by production tools such as ParaView and VisIt.
zfp	Open-source library for compressed floating-point and integer arrays that support high throughput read and write random access.
Applied Math	
AMReX	Framework for massively parallel, block-structured adaptive mesh refinement applications
Ginkgo	High-performance linear algebra library for manycore systems, with a focus on solution of sparse linear systems
MAGMA	Matrix Algebra on GPU and Multi-core Architectures (MAGMA) is a collection of next-generation linear algebra libraries for heterogeneous computing
hypre	Linear solvers library with emphasis on multigrid for structured and unstructured problems
Kokkos Kernels	On-node, portable, sparse/dense linear algebra library based on Kokkos programming model.
MFEM	Light-weight, scalable building blocks for implemeting finite element algorithms
PETSc	Suite of data structures, linear solvers, preconditioners, non-linear solvers for distributed memory scientific simulations
STRUMPACK	Solvers for dense rank-structured or sparse linear systems with support for variety of rank-structured formats
SUNDIALS	Nonlinear solvers and time integration library
SuperLU	Sparse direct solver library providing a robust solution approach for hard to solve sparse linear systems.
Trilinos	Framework with linear solvers, preconditioners, non-linear solvers, partitioning tools, and discretization libraries to support science simulations
libCEED	libCEED provides fast algebra for element-based discretizations, designed for performance portability, run-time flexibility, and clean embedding
AI/ML	
DeepHyper	Scalable neural architecture and hyperparameter optimization for deep neural networks on leadership-class machines
Tools	
ERT (Roofline)	Automates generation of roofline model for architecture-specific performance analysis and optimization
TAU	Portable profiling and tracing toolkit for performance analysis of parallel programs written in Fortran, C, C++, UPC, Java, Python.

FY24 Institute supported software stewardship recipients

PESO: Partnering for Scientific Software Ecosystem Stewardship Opportunities

About PESO

- PESO is a five-year post-ECP software-ecosystem stewardship and advancement project. In partnership with the Consortium for the Advancement of Scientific Software (CASS), PESO will establish and steward a sustainable scientific software ecosystem comprising libraries and tools that deliver the latest high-performance algorithms and capabilities for DOE mission-critical applications.

Key PESO goals

- PESO will enable applications to realize 100X improvement in both high-end capabilities and energy efficiency by leveraging accelerator devices
- PESO will emphasize software product quality, the continued fostering of software product communities, and the delivery of products, working with CASS

Key PESO Activities

- **Partnerships**: We lead CASS efforts for diverse and inclusive workforce with sustainable career paths. We shepherd BSSw Fellows Program and BSSw.io portal.
- **Services**: We provide services including software product management, integration, and delivery, as well as software quality assurance and security.
- **Products**: We deliver & support products via Spack & E4S, provide porting & testing platforms leveraged across product teams to ensure code stability & portability.

PI: Michael Heroux, Sandia National Laboratories
Collaborating Institutions: ANL, Berkeley, BNL, Kitware, LLNL, LANL, ORNL, PNNL, SNL, SHI, UO
ASCR Program: Software Stewardship and Advancement
ASCR PM: William Spotz
Resources: https://pesoproject.org, https://e4s.io, https://hpsf.io

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.

PESO is unique in its organization by composing itself of many members of other software stewardship organizations (SSOs) to best ensure tight integration across the SSOs and support the mission of the Consortium for the Advancement of Scientific Software (CASS).

PESO Partnerships, Services, and Products: A Summary

PESO: Partnering for Scientific Software Ecosystem Stewardship Opportunities

PESO Partnerships

Stakeholder Engagement and Consortium Partnerships

Consortium

- Spack support
- Products in E4S
- SW practices
- PIER activities

Applications Community

- Spack support
- E4S support

Computing Facilities

- Spack support
- E4S integration
- E4S user support

Commercial HPC Companies

- Engage in joint activities to advance the scientific software ecosystem
- Develop business models to further partnerships
- Increase release coordination activities

US Agencies

- Engage in business model discussions & plans for use of E4S
- Work with commercial providers to establish a support model
- Explore opportunities for joint product development

Industrial Users

- Engage in business model discussions & plans for use of E4S
- Work with commercial providers to establish a support model
- Explore models for mixed open-proprietary software stacks

Community Development

Broadening Participation of Underrepresented Groups in DOE Computing Sciences

- Coordinate consortium crosscutting-layer PIER planning
- Seek support for Sustainable Research Pathways Program
- Lead HPC Workforce Development and Retention Action Group

Better Scientific Software (BSSw) Fellowship Program

- Coordinate BSSw Fellowship Program – which gives recognition and funding to leaders and advocates of high-quality scientific software
- Seek sustainable support for BSSw Fellows, Honorable Mentions, travel, and program management for 2025 and beyond

PESO Services

Integration Partnerships

Provide resources and support for portfolio build, integration, and testing capabilities

- Spack integration
- CI testing
- Portfolio support & management

in collaboration with & co-funded by SSOs

- On-node & inter-node programming systems (w. S4PST)
- Math libraries, Data & viz, ML/AI (w. OASIS)
- Tools (w. STEP), Workflows (w. SWAS)
- NNSA software (funded by NNSA)

SQA & Security

Provide infrastructure to support and leverage product team SQA efforts

- Supply chain, Product quality
- Testing, Documentation

PESO Products

E4S

- Support for product integration
- E4S website
- Documentation, Training

Spack

- Features for consortium products
- Documentation, Training

Port & Test Platforms

- Frank test & development system
- Cloud resources
- Documentation, training

BSSw.io Content (w. COLABS)

- Short articles on topics related to scientific software productivity and sustainability (recruit, write, review, & edit)

Stakeholders:
Applications Community
Commercial HPC Companies
Industrial Users
US Agencies

DOE Computing Facilities:
ALCF NERSC
OLCF

CRLC: Computational Research Leadership Council: ANL, BNL, LBNL, LLNL, LANL, ORNL, PNNL, SNL

PESO Advisory Board
Reps from ANL, LBNL, LLNL, LANL, ORNL, SNL

S3C Consortium
PESO, COLABS, CORSA, OASIS, STEP, SWAS, S4PST

DOE Program Managers
ASCR: Hal Finkel, Ben Brown, Saswata Hier-Majumder, Robinson Pino, Bill Spotz, David Rabson
NNSA: Si Hammond

PESO Organizational Chart

Mike Heroux, SNL - PI **Lois Curfman McInnes, ANL - Co-PI**

PESO Partnerships

Stakeholder Engagement (Mike Heroux, SNL)

Partnerships Coordinator (Terece 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. OASIS)
- Berk Geveci, Kitware, Data and viz (w. OASIS)
- Lavanya Ramakrishnan, LBNL, Workflows (w. SWAS)
- Mahantesh Halappanavar, PNNL, AI/ML (w. OASIS)

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

- David Bernholdt, ORNL, RSE engagement (funded by COLABS)
- Addi Malviya-Thakur, ORNL, Foundation engagement (funded by CORSA)
- Elaine Raybourn, SNL, Consortium-wide community development (funded by CORSA)
- Ulrike Yang, LLNL, NNSA software (funded by NNSA)
- Partners at ALCF, NERSC, OLCF (funded by facilities, SW integration)

Community Development (Lois Curfman McInnes, ANL)

Broadening Participation Initiative

- Mary Ann Leung, Sustainable Horizons Institute, PIER planning, lead of Sustainable Research Pathways (SRP)
- Daniel Martin, LBNL, lab lead of Sustainable Research Pathways
- Suzanne Parete-Koon, ORNL, lead of HPC Workforce Development and Retention Action Group

Better Scientific Software (BSSw) Fellowship Program

- Elsa Gonsiorowski, LLNL, Coordinator of BSSw Fellowship Program
- Erik Palmer, LBNL, Deputy Coordinator of BSSw Fellowship Program

PESO Services

Integration Coordinator (Jim Willenbring, SNL)

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

- Damien Lebrun-Grandie, ORNL, On-node prog systems (w. S4PST)
- Hui Zhou, ANL, Inter-node programming systems (w. S4PST)
- Bill Hoffman, Kitware, Tools (w. STEP)
- Satish Balay, ANL, Math libs (w. OASIS)
- Patrick O'Leary, Kitware, Data & viz (w. OASIS)
- Matteo Turilli, BNL, Workflows (w. SWAS)
- Sam Browne, SNL, NNSA software (funded by NNSA)

SQA & Security (David Bernholdt, ORNL)

- Ross Bartlett (SNL)
- Berk Geveci (Kitware)
- Jim Willenbring (SNL)

PESO Products

E4S (Sameer Shende, U Oregon)

- Luke Peyralans, Erik Keever, Wyatt Spear, Jordi Rodriguez

Spack (Todd Gamblin, LLNL)

- Greg Becker, LLNL
- Tammy Dahlgren, LLNL

Port & Test Platforms (Gamblin & Shende)

- In partnership with Univ of Oregon, Cloud, etc.

BSSw.io Content (w. COLABS)

- Ross Bartlett, SNL
- Keith Beattie, LBNL
- Patricia Grubel, LANL
- Mark Miller, LLNL

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

We launched the High Performance Software Foundation (HPSF) at ISC

HIGH PERFORMANCE SOFTWARE FOUNDATION

Scientific Achievements

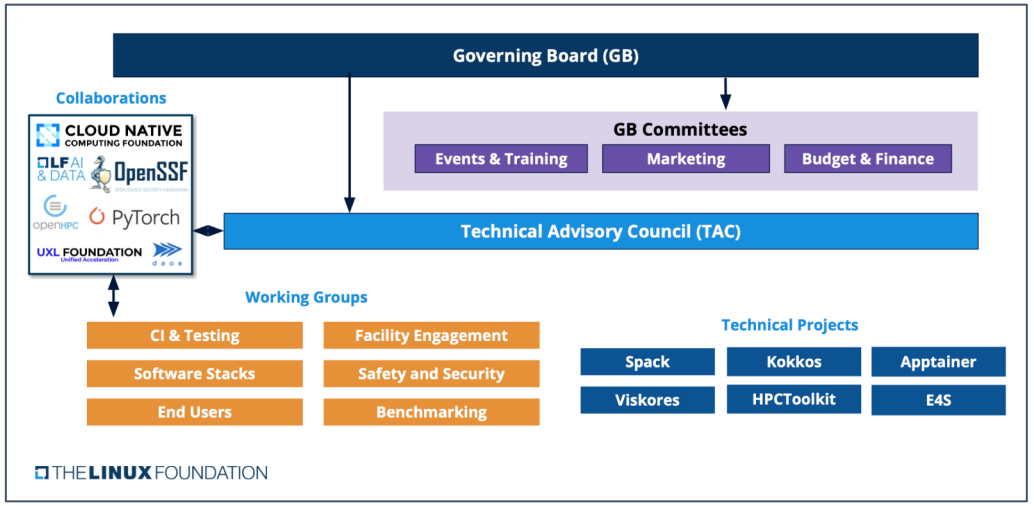
- NNSA led the formation of HPSF over the past 18 months, in close collaboration with DOE/ASCR, industry, and the Linux Foundation
- 15 founding members, 6 initial projects from industry, academia, labs around the world
- HPSF provides open source projects with:
  - A neutral home
  - Collaborations
  - Open governance
  - Funds for project infrastructure, working groups, events, other initiatives

Significance and Impact

- Initial membership raised more funds than expected: **~$1M annual budget**
- ISC kickoff BOF session was standing-room only; generating much excitement
- Expect to grow membership and projects over time
  - 2 NNSA, 2 ASCR, 2 European projects in the pipeline
  - Expecting at least 2 more general members within the year

Approach

- Separate financial (GB), technical (TAC), and project governance
- Interact directly with key projects in the HPC ecosystem
- Grow contributor base through increased adoption, training, events, outreach
- Build a portable, accelerated software stack for HPC and beyond



Premier Members

aws, Hewlett Packard Enterprise, Sandia National Laboratories, Lawrence Livermore National Laboratory

General Members

AMD, intel, NVIDIA, Argonne NATIONAL LABORATORY, OAK RIDGE National Laboratory, Los Alamos NATIONAL LABORATORY, kitware, cea

Associate Members

UNIVERSITY OF OREGON, UNIVERSITY OF MARYLAND, CDAC

PI(s)/Facility Lead(s): Todd Gamblin, Christian Trott
Collaborating Institutions: NNSA/ASC, PESO, CORSA, Linux Foundation
DOE Programs: NNSA/ASC, ASCR/NGSST
DOE PMs: Si Hammond, William Spotz, David Rabson, Hal Finkel
Resources: https://hpsf.io

National Nuclear Security Administration

S4PST – Stewardship for Programming Systems and Tools

Objective: Advancement of programming systems for the next generation high performance computing systems and its seamless integration with emerging AI technologies for science.

Description: Two-fold strategy

1. Preserve the legacy of the US Department of Energy Exascale Computing Project (ECP) critical HPC programming systems
2. Incubate the integration of HPC with the latest industry-driven AI technologies revolutionizing the broader computing landscape (e.g. large language models, LLMs).

Approach

Programming Systems are the first point of contact in human-computer interactions, and never ceased to evolve along with hardware and software technology

- Steward the legacy and strategic evolution of ECP critical programming systems
- Act upon technical, economical, and social requirements to integrate HPC and AI for science
- Provide flexibility in defining scalable activities to maximize the impact of our portfolio on ASCR
- Balance value and growth activities through coordination with ASCR stakeholders and those in the broader computing landscape.
- Provide an aggressive strategy to diversify the highly-specialized pipeline of programming systems stewards to promote inclusive and equitable research.

S4PST Product Portfolio

Product	*Product Description*	*Product Lead*	*Lead Institution*
OpenMP/OpenACC	*Portable Parallel Programming Extension and runtime for C, C++ and Fortran*	*Sunita Chandrasekaran*	*UD*
LLVM	*Focus on HPC support for the de facto standard Open-Source Compiler*	*Johannes Doerfert*	*LLNL*
Kokkos/C++	*Performance Portable Programming Systems for modern C++*	*Christian Trott*	*SNL*
Fortran	*Focus on new node parallel computing features*	*Damian Rouson*	*LBNL*
OpenMPI	*MPI implementation contributed by several institutions and vendors*	*Thomas Naughton III*	*ORNL*
MPICH	*First Open Source MPI implementation. Basis for several vendors' MPI*	*Yanfei Guo*	*ANL*
Legion	*Distributed Asynchronous Task-Parallel Runtime*	*Pat McCormick Alex Aiken*	*LANL SLAC*
UPC++ & GASNet-EX	*Alternative distributed programming model and runtime*	*Paul Hargrove*	*LBNL*
HIP	*AMD's portable accelerator programming runtime*	*Brice Videau*	*ALCF*
SYCL	*Portable modern C++ programming systems with compiler support.*	*Thomas Applencourt*	*ALCF*

STEP Overview – Software Tools for Understanding Performance and Behavior

Software Tools Ecosystem Project (STEP) – https://ascr-step.org

Scientific Achievement

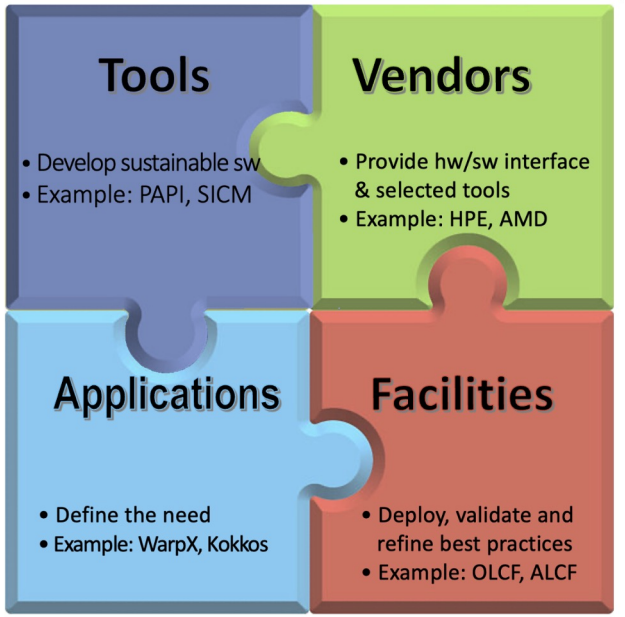
The Software Tools Ecosystem Project (STEP), a member of CASS, enables scientists, facility operators, and vendors to unlock new scientific discoveries by providing the tools necessary to understand and enhance the behavior of scientific applications at scale.

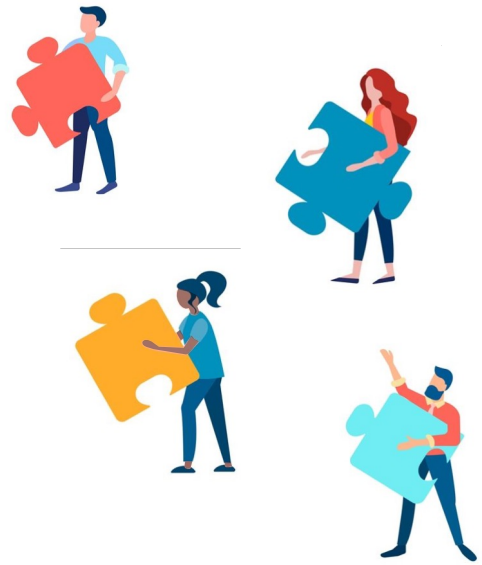
Significance and Impact

STEP provides stewardship and advancement for critical tools and supporting software that perform monitoring, analysis, and diagnosis of performance and behavior of codes. Examples include application profilers, tracing tools, system monitors, etc. As computers have increased in complexity and scale, using them effectively has become much more difficult. STEP addresses this acute need through sophisticated and openly available software.

Initial Funded Software Packages

Software Tool	PI
HPCToolkit	John Mellor-Crummey, Rice Univ.
PAPI	Heike Jagode, Univ. of Tennessee
Dyninst	Barton Miller, Univ. of Wisconsin
TAU	Sameer Shende, Univ. of Oregon
Darshan	Shane Snyder, Argonne Nat. Laboratory





Cutting edge software tools are closely bound to architectures, system software, and applications in ways that other types of software are not. STEP relies on proactive co-design of interoperable tools and deep interaction with diverse stakeholders to address this challenge. This is accomplished via recurring community meetings and input from vendor representatives, application scientists, and facility operators on the STEP Oversight Council.

STEP Consortium Leads: Terry Jones, ORNL (Director), Philip Carns, ANL (Deputy Director)
ASCR Program: Next Generation Scientific Software Technologies (NGSST)
ASCR PM: David Rabson
STEP website: https://ascr-step.org/

STEP SOFTWARE TOOLS ECOSYSTEM PROJECT

Diving in deeper – STEP's Challenges & Opportunities …

Lead PI: Terry Jones
Deputy PI: Phil Carns

Software Tools Ecosystem Project (STEP) – https://ascr-step.org

Objectives and Scope

- Tools and supporting software for monitoring, analysis, and diagnosis of performance and behavior of codes on advanced computing systems.
- Examples: application profilers, tracing tools, system monitors, etc.
- Co-design with hardware vendors, application developers, facilities and tool developers.

Challenges

- These tools rely on a deep understanding of hardware, and hardware is rapidly changing.
- Vendors are reluctant to divulge hardware details.
- Stakeholders are very diverse and currently have insufficient communication paths.

Opportunities

- STEP can be a vehicle to improve communication among tool developers, application teams, vendors and facilities.
- STEP can be a clearing-house for efficiently managing critical HPC technology.
- STEP can be a resource for workforce development.

An interesting fact about STEP. . .

- Tools are closely bound to architectures and system software in ways that other types of software, such as libraries and scientific applications, are not.
- For example, a tool that tracks how an application uses computing resources must be able to measure low-level architectural events and metrics and relate them to program progress and source code.
- The need for tools is most acute for understanding code performance on systems that push the boundaries of technology and scale, but these systems' novelty makes them extremely difficult for tool developers to support when first deployed.

https://ascr-step.org

Enabling scientific productivity with TAU — a STEP software tool

Software Tools Ecosystem Project (STEP) – https://ascr-step.org

Scientific Achievement

The Software Tools Ecosystem Project (STEP), a charter member of the Consortium for the Advancement of Scientific Software (CASS), enables scientists, facility operators, and vendors to unlock new scientific discoveries by providing the tools necessary to understand and enhance the behavior of scientific applications at scale. In one example (see image at right), STEP tools led directly to a 3.8x faster time to solution for a key chemistry application.

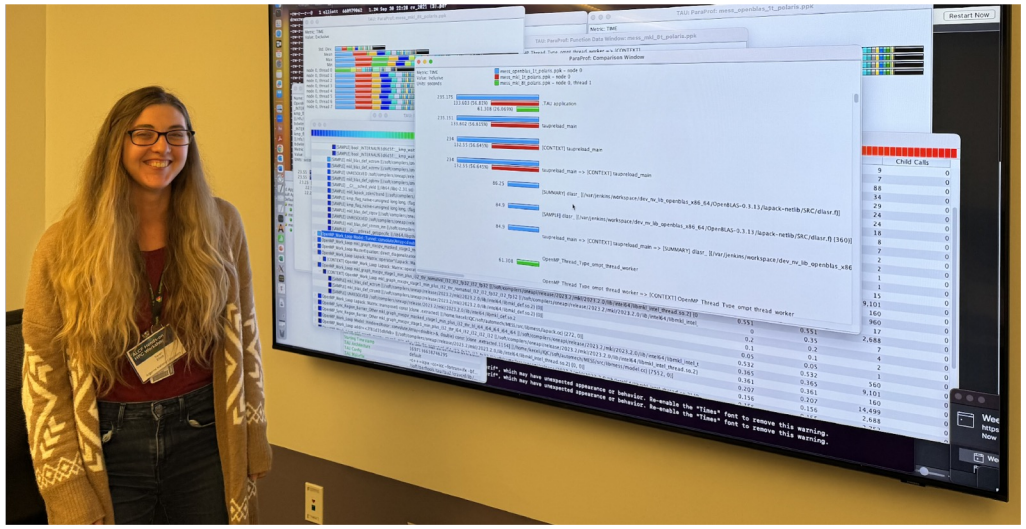
Significance and Impact

Stewardship and advancement of software tools protects and maximizes the investment in scientific computing by ensuring optimal use of current and future computing technologies. This effort impacts the full range of scientific domains and computing platforms supported by the DOE.

Technical Approach

- Stewardship and advancement of a critical portfolio of software tools.
- Delivering technology directly to scientists via interactive hands-on training.
- Leverage guidance from application developers, facility operators, and commercial vendors via the STEP Oversight Council.
- Work with CASS to coordinate and amplify community impact.

STEP Consortium Leads: Terry Jones, ORNL (Director), Philip Carns, ANL (Deputy Director)
TAU Software Tool Lead: Sameer Shende, U. of Oregon
Training Collaborator: Suzanne Parete-Koon (ORNL)
ASCR Program: Next Generation Scientific Software Technologies (NGSST)
ASCR PM: David Rabson
Training website: https://ascr-step.org/training



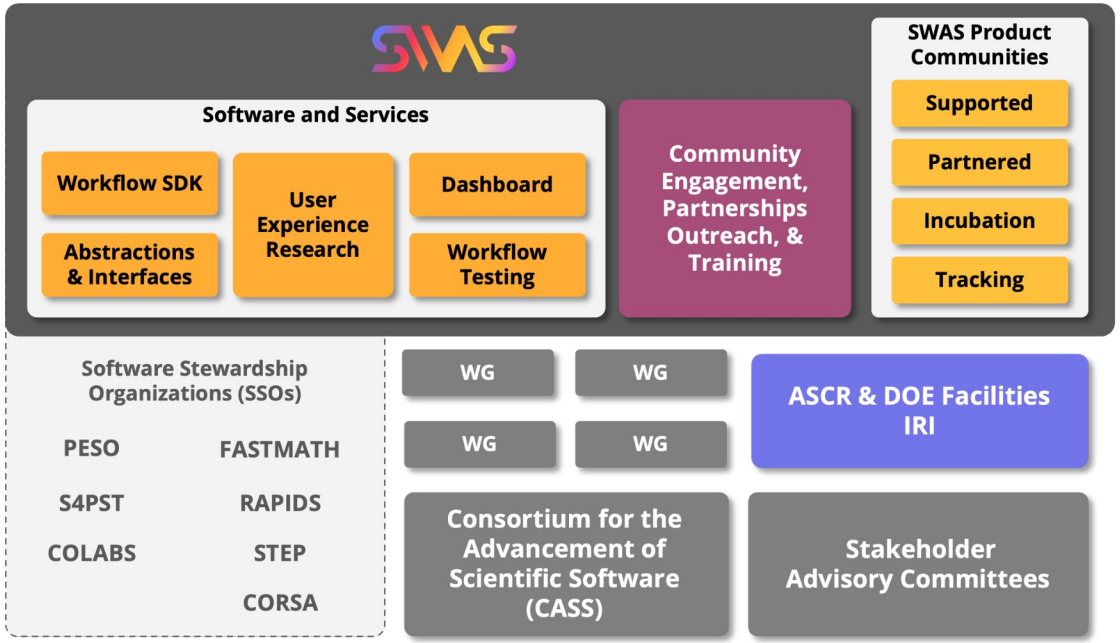
Chemist Sarah Elliott of Argonne National Laboratory at the ALCF Hands-on HPC Workshop (October 10-12, 2023), where she worked with Professor Sameer Shende of University of Oregon and STEP to visualize and optimize the performance of the MESS computational chemistry application. MESS is notably a mature application that has received much attention to performance since its inception in 2013. The result of this recent collaboration between scientists and tool developers was 3.8x faster time to solution for a critical simulation.

STEP SOFTWARE TOOLS ECOSYSTEM PROJECT
Tuning and Analysis Utilities
UNIVERSITY OF OREGON
Argonne NATIONAL LABORATORY

SWAS: Stewardship and Advancement of Workflows and Application Services

Objective

SWAS is a pivotal initiative addressing the complex **workflow** needs of the **DOE science community**. It aims to centralize activities around workflow software, including *research*, *development*, *education*, and *training*. By focusing on simulations, real-time data analysis, and AI/ML integration, SWAS seeks to overcome the fragmentation and inefficiencies in the current scientific workflow ecosystem. Its mission is to steward, support, and advance critical **workflow software and services** across all DOE science disciplines.



Significance and Impact

SWAS targets enhancing core capabilities widely required by the community and aims to foster robust community engagement, partnerships, outreach, and training initiatives. SWAS is necessary to bringing the IRI's strategic vision to fruition by supporting the essential software infrastructure and services needed to integrate computational and experimental research facilities seamlessly. SWAS is a vital bridge between ASCR computing facilities and research and software development efforts, enhancing the DOE's capacity to tackle pressing scientific challenges through improved computational efficiency and innovation.

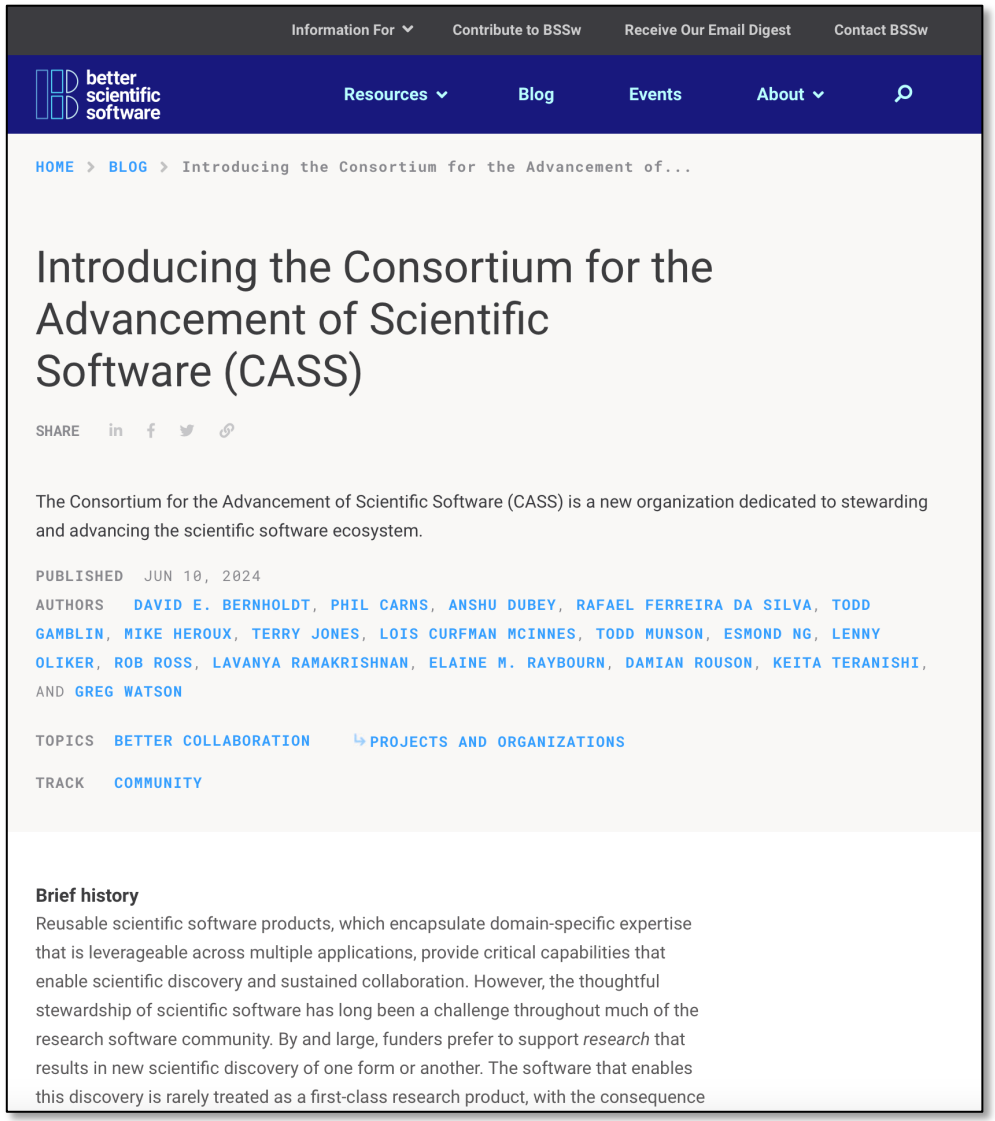
Technical Approach

- ***Community Engagement and Workforce Development:*** SWAS prioritizes building a vibrant, engaged community. It focuses on workforce support, disseminating best practices, and training initiatives to cater to the diverse research needs across DOE science disciplines.

- ***Software Evaluation and Lifecycle Management***: SWAS will employ workflow-specific metrics for evaluating software, ensuring its relevance and efficacy in addressing the dynamic requirements of scientific research. Our active participation in the governance of the S3C ecosystem is pivotal to not only facilitate the continuous adaptation and improvement of the workflow ecosystem but also underscores our dedication to supporting the DOE's mission to lead in scientific innovation.

- ***Support for Critical Workflow Software:*** By identifying and supporting software that offers core capabilities essential to the scientific community, SWAS addresses the diverse needs of scientific workflows, from simulation orchestration to data analysis and AI/ML.

CASS: More info



- Please consider telling us something about yourself and your interests in CASS: https://tinyurl.com/2024-CASS-BOFS
- CASS members provide various libraries and tools for scientific computing applications. Please select areas of interest to you (if any)
  - Programming systems
  - Performance tools
  - AI packages
  - Math packages
  - Data and viz packages
- CASS members provide community-wide interactions related to the advancement of scientific software. Please select areas of interest to you (if any)
  - Curating and delivery of scientific software ecosystems
  - Workforce development
  - Software quality and security
  - User and developer experience
  - Preparing for modern high-performance computing systems
- Please provide any other comments or suggestions. Thank you!

https://bssw.io/blog_posts/introducing-the-consortium-for-the-advancement-of-scientific-software-cass

Consortium for the Advancement of Scientific Software (CASS) Workforce Initiative

BOF: June 12, 3 pm ET: Building an Inclusive and Productive Community from Many Organizations to Support Software Stewardship

U.S. DEPARTMENT OF ENERGY | Office of Science

Partnership with
Sustainable Horizons Institute
https://shinstitute.org

SUSTAINABLE HORIZONS INSTITUTE

CASS

Fostering and stewarding a workforce community with broad pathways to sustainable HPC & AI careers

Intro to HPC & AI for Science

Accessible introductory material addressing gaps in — and expanding the pipeline of — people with foundational HPC and AI skills. This onramp begins a pathway to build experience and interest in HPC and AI for science.

Sustainable Research Pathways

A multi-lab workforce development program with students and faculty working side-by-side with DOE lab teams on world-class projects using HPC and AI for science.

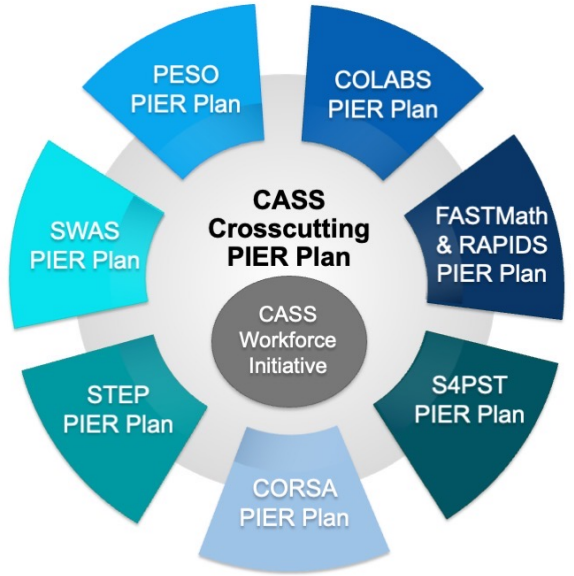
HPC Workforce Community Group

Enabling staff of DOE national labs to share their collective insight for inclusive and equitable workforce development and retention for careers in HPC and AI for science.

CASS Workforce Initiative pursues a multi-layered strategy, with both crosscutting and project-specific activities

Building on and extending the ECP Broadening Participation Initiative:

- *Building a diverse and inclusive HPC community for mission-driven team scienc* IEEE CiSE, Nov 2023, https://doi.org/10.6084/m9.figshare.24563371
- *Intro to HPC Bootcamp: Engaging new communities through energy justice projects*, J. Comp. Science Edu., 2024 https://doi.org/10.22369/issn.2153-4136/15/1/10
- *A multipronged approach to building a diverse workforce and cultivating an inclusive professional environment for DOE high-performance computing*, 2021, https://doi.org/10.6084/m9.figshare.17192492



Why the CASS Workforce Initiative? Unique multilab partnership across DOE computing sciences

- Strength in spanning multiple institutions / strength in numbers / network beyond what any individual lab could do
- Proactive outreach and deployment of DOE scientific software tools and technologies to communities beyond traditional targets

Discussion, Q&A