DOE/ASCR Computer Science Principal Investigators (PI) Meeting, 21-22 July 2026, Rockville, Maryland

The Consortium for the Advancement of Scientific Software (CASS): Software Stewardship for DOE/ASCR

https://cass.community/

CASS Officers			CASS Steering Committee Members					
David E. Bernholdt (ORNL)	Chair		Greg Watson (ORNL)	CORSA	Jim Willenbring (SNL)	PESO	Seyong Lee (ORNL)	S4PST
Jim Willenbring (SNL)	Vice-Chair		Todd Munson (ANL)	FASTMath	Berk Geveci (Kitware)	RAPIDS	Terry Jones (ORNL)	STEP
Elaine M. Raybourn (UCF)	Secretary		Miro Stoyanov (ORNL)	LEADS				

What Is CASS?

- A **federation of member organizations** supporting specific communities or providing crosscutting capabilities related to **scientific software stewardship**
  - Software stewardship organizations (SSOs), for short
- CASS is a vehicle for SSOs to **coordinate and collaborate** on activities that benefit the scientific software community, including developers, users, and other stakeholders
  - Common identity/"brand" gives greater visibility to our efforts in the larger community
- Currently targeting the ASCR scientific software ecosystem
  - Especially software developed/enhanced through the ECP
  - Current CASS software portfolio: https://cass.community/software/

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

Abstract

Historically, the DOE-led high-performance computing (HPC) software ecosystem has enabled scientific discovery across many fields. As AI increasingly accelerates science, robust and reusable scientific software becomes even more important—both for advancing HPC modeling and simulation and for informing trustworthy AI-based models.

The Consortium for the Advancement of Scientific Software (CASS, https://cass.community) is a federation of seven software stewardship organizations funded by DOE/ASCR's Next-Generation Scientific Software Technologies (NGSST) and Scientific Discovery through Advanced Computing (SciDAC) programs. Building on advances from the Exascale Computing Project, the CASS portfolio includes libraries and tools that underpin modern HPC modeling and simulation and connect them with AI-enabled workflows. These include scalable mathematical libraries; tools for data analysis, visualization, and management; software development and performance tools; and tools that support both AI-methods research and research using AI methods. Together, this curated software ecosystem supports a broad range of computational science applications.

CASS helps its member organizations coordinate across the ecosystem, increase the visibility of their work, and strengthen the collective value of DOE-supported scientific software. Its activities include inward-facing efforts that enhance stewardship of specific software products; outward-facing efforts that help products reach and engage users; stakeholder-facing engagement with computing facilities and vendors; and cross-cutting activities such as webinar series, community resources, and support for DOE's HPC and AI software workforce. Through this coordinated stewardship model, CASS advances the software infrastructure, community practices, and workforce capacity needed for trustworthy scientific computing in an AI-enabled future.

CASS Activities

Inward-facing activities to support and enhance specific software products

- Improving software development practices, sustainability, quality, trustworthiness, impact
- Improving user experience, integration into the larger ecosystem

Outward-facing activities to

- Curate the collection of software products (e.g., through E4S)
- Help the community find and use software that might benefit them
- Help teams find and engage with users (e.g., CASS Community BoF Days, CASS at Supercomputing, etc.)

CASS at Supercomputing

- Many events organized by CASS members and software teams at Supercomputing conferences
  - Tutorials
  - Workshops
  - Presentations
  - Papers
  - Posters
  - Booth talks
  - Birds of a Feather (BoF) sessions
- More than 50 events at SC25!

CASS Community BoF Days

- Community-led birds-of-a-feather (BoF) sessions, organized by CASS
- Annual online event, usually in February
- Teams and stakeholders **meet, learn, discuss**
  - BOFs on CASS-member **scientific libraries, tools**
  - BOFs on **community development efforts**
  - *Not limited to CASS software teams or communities*
- CASS Community BoF Days 2025
  - 15 sessions, held over three days
  - 780 total registrations

Stakeholder-facing activities to

- Facilitate the deployment of CASS software products via E4S and Spack through engagement with computing facilities
- Engage with HPC hardware, software, and service vendors to increase awareness and adoption of CASS software products
- Working groups bring together interested parties on various topics
  - Working groups are the primary means by which we organize members of the CASS community to advance our stewardship efforts
  - Most CASS working groups welcome public participation

Active Working Groups

Impact Framework
Curating the CASS Impact Framework process

Integration
Improving quality, sustainability, and interoperability across the scientific software ecosystem

Metrics
Curating and developing metrics for understanding software sustainability, quality and impact

Software Ecosystem
Planning and executing activities that support and enhance holistic collaboration across the breadth of the CASS community member organizations to sustain and advance our software libraries and tools usage as a curated portfolio

User-Developer Experience
Promote improved user-developer experiences

Workforce
Advancing the multidisciplinary community and workforce for next-generation computing sciences, with emphasis on scientific software

Supportive and crosscutting activities, including

- Resources to improve software development practices through:
  - HPC Best Practices webinar series,
  - User/Developer Experience webinar series,
  - Better Scientific Software information site,
  - …
- Advancing the multidisciplinary community and workforce for next-generation computing sciences
- The Better Scientific Software Fellowship program

Engage with CASS!

- **Participate!**
  - HPC Best Practices webinar series, UDX webinar series
  - Community BoF Days, CASS @ Supercomputing
  - Read and contribute to the Better Scientific Software resource site (https://bssw.io)
  - Apply for the Better Scientific Software Fellowship (https://bssw.io/fellowship/)
- Join our **announcement mailing list** to follow our activities and our **Slack** to engage with the CASS community
  - Links in footer of https://cass.community
- Find out more about our **software products**
  - https://cass.community/software/
- Reach out to **member organizations** in your communities of interest
  - https://cass.community/about/#current-members-and-leadership
- Participate in (or start!) **working groups**, building throughout the ecosystem
  - https://cass.community/working-groups/
- If you're a commercial vendor in the scientific computing space, join our **Vendor Forum**
  - https://cass.community/vendor-forum/
- **Join CASS** and help us reach a larger portion of the scientific software ecosystem!
  - Email cass-steering-committee@email.ornl.gov

CASS Software Portfolio

- Currently, stewardship efforts are explicitly supported for a portion of the ASCR scientific software ecosystem
  - Evolves over time
- Building on advances from the Exascale Computing Project (ECP)
- Includes libraries and tools that underpin modern HPC modeling and simulation and connect them with AI-enabled workflows
- *Note: software packages may fall into more than one of the areas listed*

AI Building Blocks

Provide capabilities often used in artificial intelligence-based workflows

- AMReX, libEnsemble, PETSc/TAO, PyTUQ

Artificial Intelligence

Directly support artificial intelligence research and research using artificial intelligence

- CESAR, DeepHyper, EXARL, Fiats, GenAI4UA, libROM, NeuroMANCER, Onieus, StFT

Data and Visualization

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

- ADIOS, Ascent, ChatVis, DIY, HDF5, Oineus, ParaView, ParaView Catalyst, PnetCDF, VisIt, Viskores, zfp

Development Tools

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

- AML, Chimbuko, CodeScribe, Darshan, Dyninst, Empirical Roofline Toolkit, HPCToolkit, Julienne, PAPI, TAU, ytopt

Mathematical Libraries

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

- AMReX, Dakota, FASTEig, hypre, Kokkos Kernels, libEnsemble, MFEM, PETSc/TAO, PUMI Components, PyTUQ, STRUMPACK, SUNDIALS, SuperLU

Programming Models and Runtimes

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

- Caffeine, chipStar, GASNet, Kokkos, Legion, LLVM Flang, MPICH, Open MPI, OpenACC Verification and Validation Suite, OpenMP Verification and Validation Suite, UPC++

Software Ecosystem and Delivery

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

- E4S, Spack

Uses AI

Use artificial intelligence techniques internally

- ChatVis, Chimbuko, CodeScribe, FASTEig, ytopt

Science Impacts of CASS Software
(A Few Examples)

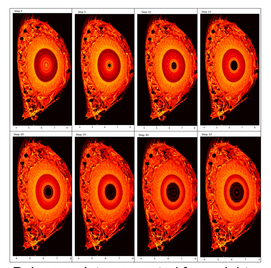
Whole Device Modeling of Magnetically Confined Fusion Plasma

The fusion community is developing an approach to first-principles-based whole device modeling that will provide predictive numerical simulations of the physics required for magnetically confined fusion plasmas to enable design optimization and fill in the experimental gaps for ITER and future fusion devices

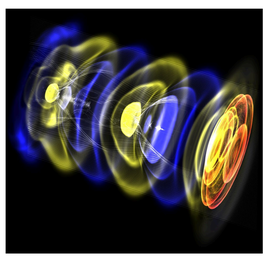
The following software was used by the WDMApp project for whole-device modeling

- Mathematical libraries: PETSc/TAO, hypre, SuperLU, AMReX, MFEM, SUNDIALS, Kokkos Kernels, STRUMPACK, libEnsemble
- Software ecosystem and delivery: Spack, E4S
- Data and visualization: ADIOS, HDF5, PnetCDF, zfp, Viskores, DIY
- Programming models and runtimes: Kokkos, Open MPI, MPICH, OpenMP V&V Test Suite, OpenACC V&V Test Suite
- Development tools: TAU, HPCToolkit, PAPI, Darshan

- DOI:10.1063/5.0027160



Poincare plots generated from eight different time steps from a run of WDMApp's XGC code on Frontier. Attribution: ORNL: David Pugmire, Kenneth Moreland, Jong Choi, Scott Klasky. PPPL: Chong-Seock Chang, Seung-Hoe Ku, Robert Hager.



Impact of AMReX integration with WarpX: Simulation of laser wakefield acceleration performed with WarpX. Image courtesy of Maxence Thévenet & the WarpX team. Description from AMReX image gallery.

WarpX Enables Computational Design of Next-Generation Plasma-Based Accelerators

WarpX is a particle-in-cell (PIC) simulation code that simulates particles that interact with each other, and with electromagnetic fields and surfaces. Originally developed to model chains of plasma-based particle accelerators for future high-energy physics colliders, its domain of applications has broadened to other topics that include the modeling of other types of particle accelerators and beam physics, laser-plasma interactions, astrophysical plasmas, nuclear fusion energy and plasma confinement, plasma thrusters and electric propulsion, and microelectronics

The following software was used by the WarpX project

- Mathematical libraries: AMReX, libEnsemble
- Software ecosystem and delivery: Spack, E4S
- Data and visualization: ADIOS, HDF5, ParaView, Ascent, VisIt, Viskores
- Programming models and runtimes: Open MPI, MPICH
- Development tools: Darshan, Empirical Roofline Toolkt, PAPI

- DOI:10.1109/SC41404.2022.00008