# Overview of SUNDIALS

Consortium for the Advancement of Scientific Software (CASS)
BoF Days, 2026

Feb. 12, 2026

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In collaboration with the SUNDIALS team: Cody J. Balos (LLNL), David J. Gardner (LLNL), Dan Reynolds (UMBC), Steven B. Roberts (LLNL)

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BOF Days

February 10 - 12, 2026

https://cass.community

# The Consortium for the Advancement of Scientific Software (CASS)

CASS

BOF DAYS

https://cass.community/news/2026-02-10-cass-bof-days.html

# CASS: Stewardship and Advancement of the Scientific Software Ecosystem

- **Inward-facing activities:** Strengthening software products
  - Improve development practices, sustainability, quality, and trustworthiness
  - Enhance user experience and integration within the broader ecosystem
- **Outward-facing activities:** Community engagement and discovery
  - Curate and evolve the software portfolio
  - Help teams connect with and grow their user communities
  - Enable the broader community to discover and adopt useful software

CASS Members

**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

Sponsored by the Department of Energy, Office of Advanced Scientific Computing Research

# Engage with CASS!

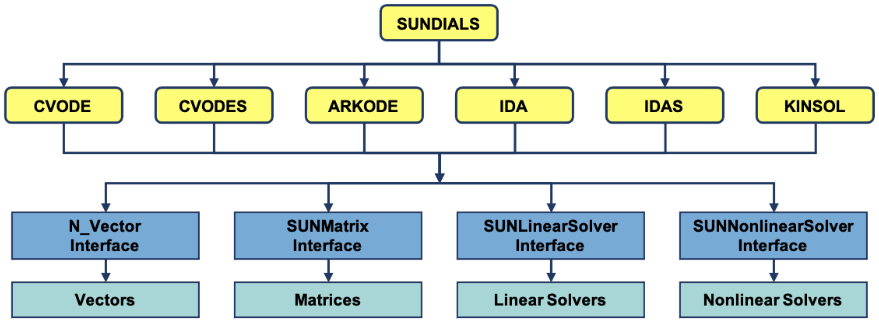
- Learn about CASS:
  - https://cass.community/about/
- Join the CASS Announcement list (low-volume):
  - http://eepurl.com/iRiSnY
- Find out more about our **software products**
  - Catalog: https://cass.community/software/
  - Collected as part of the Extreme-Scale Scientific Software Stack (E4S)
- Participate in **CASS Working Groups**
  - Impact Framework, Integration, Metrics, Software Ecosystem, User-Developer Experience, Workforce
  - https://cass.community/working-groups/

# BoF Session Outline

- “Overview of SUNDIALS,” Carol Woodward (LLNL)
- “New Features in SUNDIALS,” Daniel Reynolds (UMBC)
- “Python Interfaces in SUNDIALS,” David Gardner (LLNL)
- “Using SUNDIALS to Efficiently Drive Time-Integration in AMReX-Based PDE Solvers,” Andy Nonaka (LBNL)
- “Dynamics of atomic nuclei with SUNDIALS,” Francesca Bonaiti (MSU)
- “Towards near-real-time discontinuous Galerkin gyrokinetic simulations of fusion plasmas: collisions via super time stepping,” Manaure Francisquez (PPPL)
- “Integrating SUNDIALS into MATLAB,” Brett Buckner (Mathworks)
- Discussion
  - New or interesting uses of SUNDIALS
  - Identify features needed for further SUNDIALS development
  - Share successes and failures of SUNDIALS uses among applications

# SUite of Nonlinear and DIfferential-ALgebraic Solvers

- SUNDIALS is a software library consisting of ODE and DAE integrators and nonlinear solvers
- Written in C with interfaces to Fortran and Python
- New interfaces in Matlab starting with release R2024a
- Designed to be incorporated into existing codes
- Includes a rich infrastructure of support on exascale systems and applications
- Freely available; released under the BSD 3-Clause license ( >100,000 clones/downloads per year)
- Active user community supported by sundials-users email list
- Detailed user manuals included with each package and online at https://sundials.readthedocs.io



- Nonlinear and linear solvers and all data use is fully encapsulated from the integrators and can be user-supplied
- All parallelism is encapsulated in vector and solver modules and user-supplied functions

**https://computing.llnl.gov/casc/sundials**

# SUNDIALS brings methods to nonlinear time dependent systems

- CVODE, IDA, and sensitivity analysis variants (forward and adjoint), CVODES and IDAS, use linear multistep methods
  - CVODE solves ODEs, $\dot{y} = f(t, y)$
  - IDA solves DAEs, $F(t, y, \dot{y}) = 0$
  - Adaptive in both order and step sizes; include event detection
  - Both packages include stiff BDF methods; CVODE includes nonstiff Adams-Moulton methods
- ARKODE provides adaptive one-step, multistage time integration methods
  - Solves $M\dot{y} = f_I(t, y) + f_E(t, y), \quad y(t_0) = y_0 \quad M(t)$: any nonsingular (optionally time-dependent) mass matrix
  - Supports adaptive time steps through multistage embedded methods
  - Six steppers:
    - ARKStep: explicit, implicit, and additive ImEx Runge-Kutta methods; with adaptivity, event detection, etc.
    - ERKStep: streamlined explicit RK implementation
    - LSRKStep: Low storage explicit RK methods
    - MRIStep: multirate infinitesimal step methods
    - SplittingStep: Operator splitting methods (low and high order)
    - SPRKStep: symplectic explicit RK for partitioned Hamiltonian systems (conserves energy or similar quantities)
  - Parallel-in-Time support: XBraid wrappers for SUNDIALS vectors and explicit, implicit, and ImEx methods in ARKStep
- KINSOL solves nonlinear algebraic systems with Newton or accelerated fixed point methods

# What are some of the newer features in SUNDIALS?

- **Command line control over SUNDIALS options** - enables the use of AI/ML tools to tailor SUNDIALS options to a specific application and improve performance
- **Low storage RK methods** along with dominant eigenvalue estimation including both Power iteration and Arnoldi dominant eigenvalue estimation options provided
- **An interface to batched, iterative, linear solvers from the Ginkgo library** - allows any batched solver in Ginkgo to be utilized
- **Discrete adjoints for explicit methods in ARKStep and ERKStep**
- **Python interfaces** to enable greater SUNDIALS use in the Python and ML/AI communities, with zero copy data exchange
- **Operator splitting** module with arbitrary order methods

# What are we working on now?

- Discrete adjoint capability for explicit multirate RK methods in ARKODE (with constant time steps)
- Complex vector and data structure support
- Embedded SSP ImEx methods
- Automatic switching between Newton and fixed point solvers for problems that change stiffness

# Where to learn more and get the software

Visit the SUNDIALS website: https://computing.llnl.gov/sundials

See presentations list at the SUNDIALS publications page: https://computing.llnl.gov/sundials/publications

Visit the SUNDIALS GitHub page: https://github.com/LLNL/sundials

Clone the repository or download the tarball from the SUNDIALS GitHub page and build with CMake: https://github.com/LLNL/sundials/releases

Detailed user manuals online: https://sundials.readthedocs.io

Install SUNDIALS using Spack: “spack install sundials”

**https://computing.llnl.gov/sundials**

# SUNDIALS Team

Current Team:

Cody Balos

David Gardner

Dan Reynolds

Steven Roberts

Carol Woodward

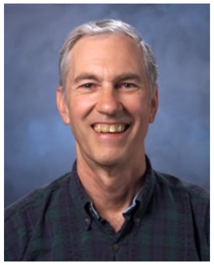
PostDocs (UMBC):

Mustafa Ağgül

Sylvia Amihere

Yifan Hu

Alumni: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**computing.llnl.gov/sundials**

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