

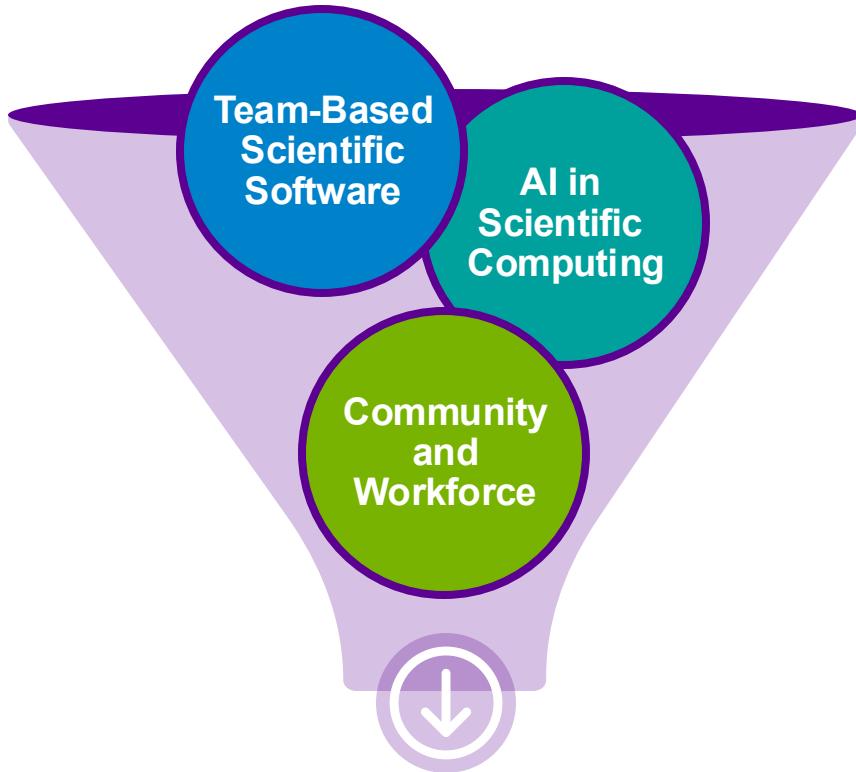
# Toward Next-generation Ecosystems for Scientific Computing

**Harnessing community,  
software, and AI for cross-  
disciplinary team science**

April 29 – May 1, 2025  
Chicago, IL

## Workshop Organizers:

**Lois Curfman McInnes**, Argonne National Laboratory  
**Dorian Arnold**, Emory University  
**Prasanna Balaprakash**, Oak Ridge National Laboratory  
**Mike Bernhardt**, Team Libra  
**Beth Cerny**, Argonne National Laboratory  
**Anshu Dubey**, Argonne National Laboratory  
**Denice Ward Hood**, University of Illinois Urbana-Champaign  
**Mary Ann Leung**, Sustainable Horizons Institute  
**Olivia B. Newton**, University of Montana  
**Stefan Wild**, Lawrence Berkeley National Laboratory



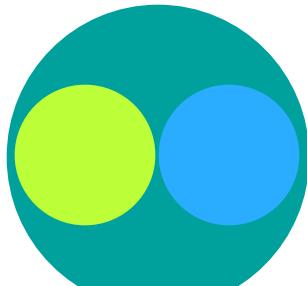
## NEXT-GENERATION ECOSYSTEMS FOR SCIENTIFIC COMPUTING

Workshop Report: <https://doi.org/10.48550/arXiv.2510.03413>

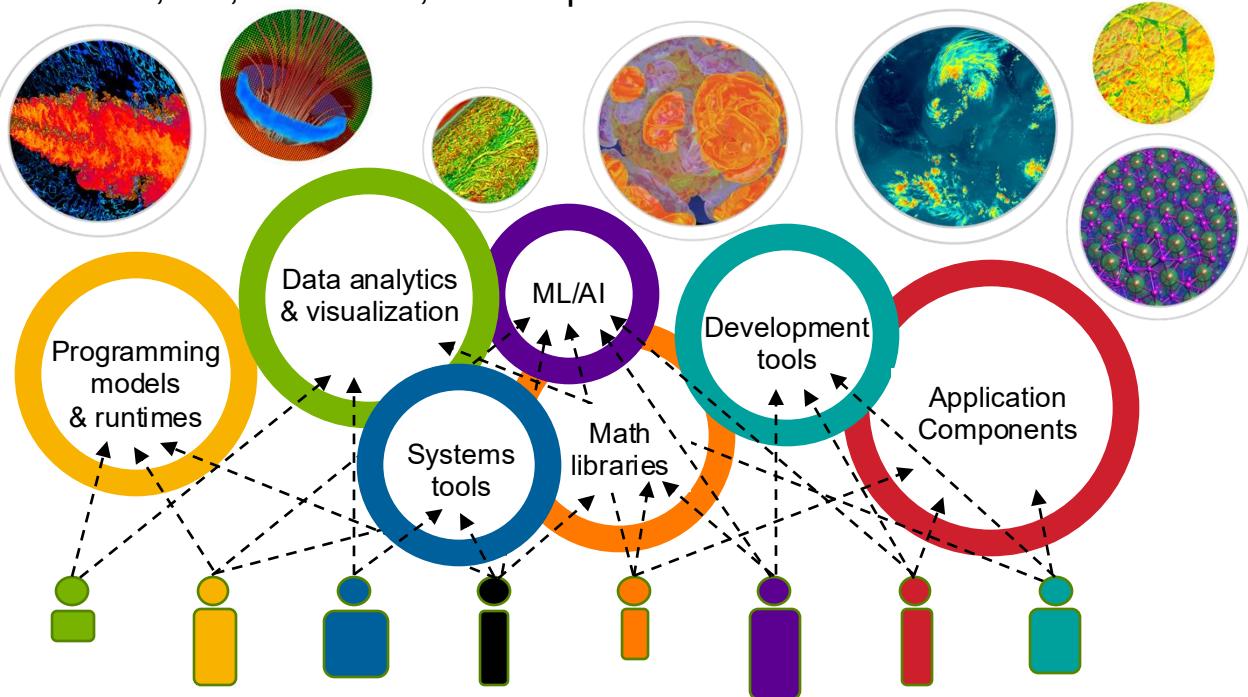
# REUSABLE SOFTWARE LIBRARIES AND TOOLS

... provide the foundation of many scientific simulations

Single small team

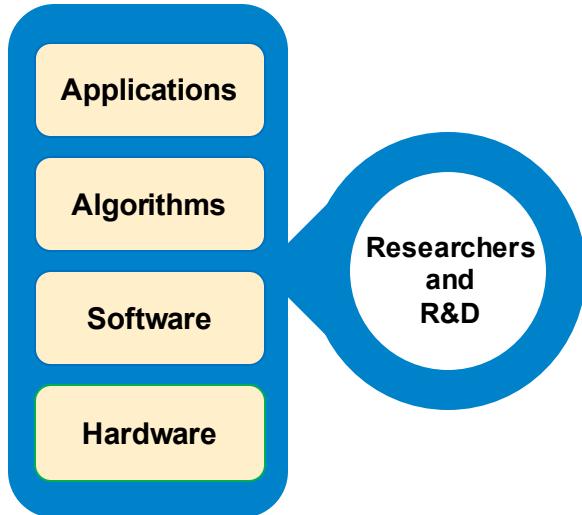


Multiphysics simulation requires expertise across science domains, math, CS, and ML/AI, all encapsulated in software

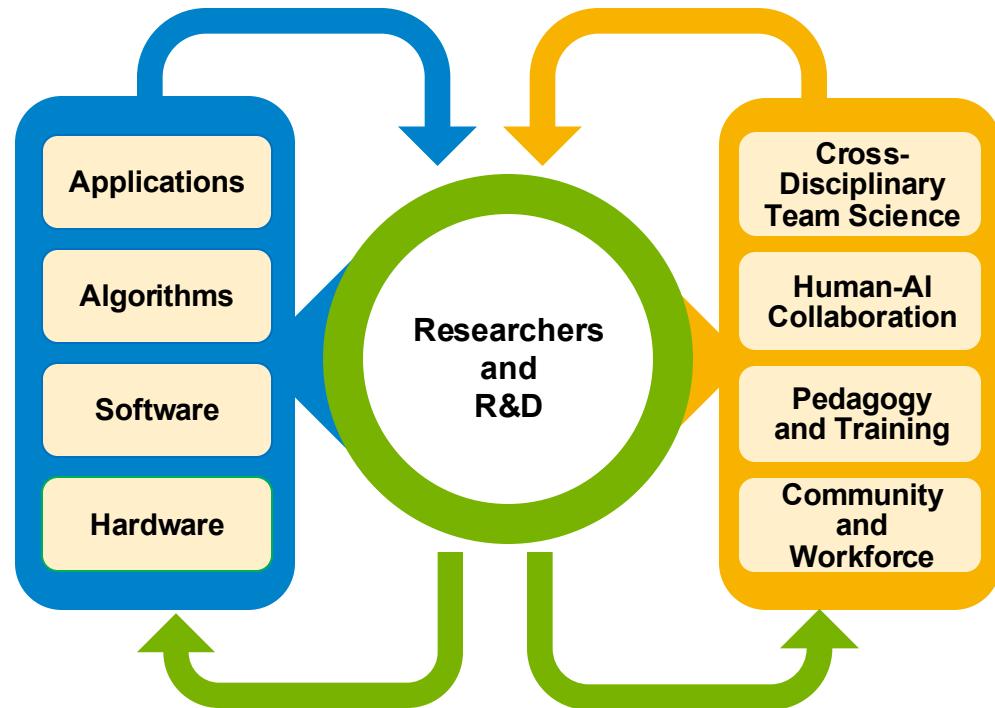


# SOCIO-TECHNICAL CO-DESIGN

Traditional co-design  
for scientific computing



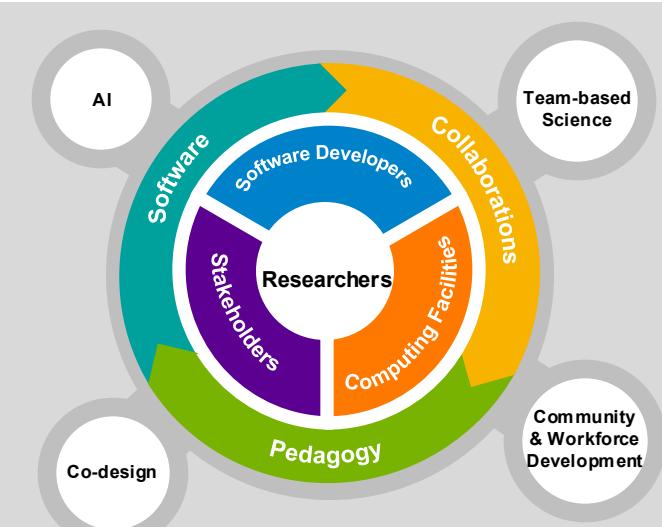
Socio-technical co-design for future  
scientific computing



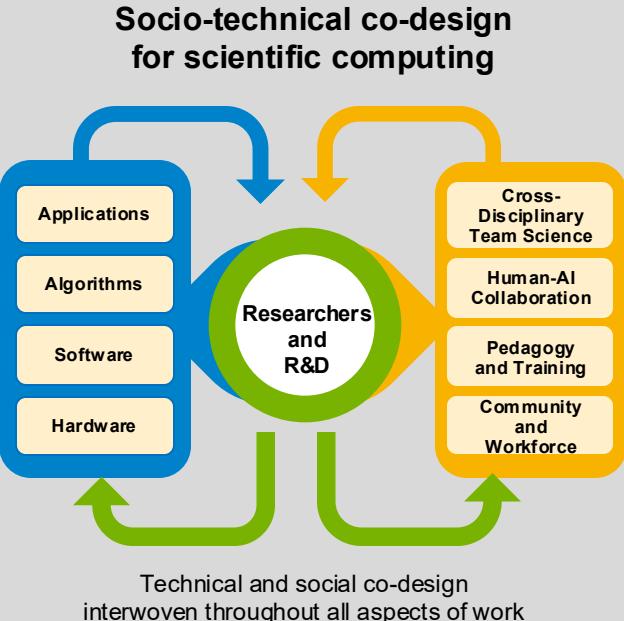
Technical and social co-design interwoven throughout all aspects of work

# WORKSHOP REPORT, SEPT 2025

## Next-Generation Ecosystems for Scientific Computing: Harnessing Community, Software, and AI for Cross-Disciplinary Team Science



As motivated by the needs of team-based science in an AI-driven future, we must advance software, cross-disciplinary collaboration, and pedagogy through co-design ... All while developing workforce and community.



### Toward Next-Generation Ecosystems for Scientific Computing

Harnessing community, software, and AI for cross-disciplinary team science

September 2025

```
xflux(F01DENS_FLUX:F0SENER_FLUX,i,j,k) = &
xflux(F01DENS_FLUX:F0SENER_FLUX,i,j,k) &
+CV1SC(/U(DENS_VAR,i-1,j,k) -U(DENS_VAR,i-1,j,k)
+U(DENS_VAR,i-1,j,k) +U(VELX_VAR,i-1,j,k) -U(DENS_VAR,i-1,j,k)
+U(DENS_VAR,i-1,j,k) +U(VELZ_VAR,i-1,j,k) -U(DENS_VAR,i-1,j,k)
+U(DENS_VAR,i-1,j,k) +U(ENER_VAR,i-1,j,k) -U(DENS_VAR,i-1,j,k)
+U(MAG_MHD) || defined FLASH_UGLM_MHD) &
xflux(F07MAG_FLUX:F0BMAGZ_FLUX,i,j,k) = &
xflux(F07MAG_FLUX:F0BMAGZ_FLUX,i,j,k) &
+CV1SC(/U(MAG_VAR,i-1,j,k) ,U(MAGZ_VAR,i-1,j,k)
-U(MAGZ_VAR,i-1,j,k)
```

ANL-25/47

### WORKSHOP PARTICIPANTS OVERVIEW

Expertise in high-performance computing (HPC), AI, computational science, applied math, computer science, research software engineering, cognitive and social sciences, community development, and more ...

- DOE lab staff: representing all 8 labs in the CRLC
  - ANL, BNL, LBNL, LLNL, LANL, ORNL, SNL
- Universities: representing 12 institutions
  - Boston Univ., Caltech, Emory Univ., Miami Univ., Texas State Univ.
  - The George Washington Univ., Univ. of Central Florida
  - Univ. of Illinois Urbana-Champaign, Univ. of Montana
  - Univ. Notre Dame, Univ. of Pittsburgh, Univ. of Texas at Austin
- Agencies, industry, small businesses, nonprofits:  
9 groups
  - DOE Office of Advanced Scientific Computing Research
  - National Academies of Sciences, Engineering and Medicine
  - Center for Scientific Collaboration and Community Engagement
  - National Science Foundation
  - Ford Motor Company
  - GE Aerospace
  - Sustainable Horizons Institute
  - TensorFlow
  - US-RSE