

Computing in Science and Engineering (CiSE)

Introduction to Accelerating Scientific Discovery With Reusable Software, Scott Lathrop, Mike Folk, Daniel S. Katz, Lois Curfman McInnes, Andy Terrel, *Computing in Science & Engineering*, 2019, Volume 21, Issue 2

Goals

- Raise awareness about reusable software among computational- and data-enabled researchers
- Identify the challenges and opportunities facing the community
- Document high-quality, sustainable, reusable software to enhance quality and reproducibility
- Identify the benefits of reusable software that follow standards of quality and good practices
- Foster communities of practice

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Papers

- A survey of organizational efforts for developing better scientific software (Katz et al.)
- Best practices for developing reusable software for geophysics, and building the CIG community of practice (Kellogg et al.)
- A component-based programming paradigm for building and using reusable software (Lanore)
- Computational chemistry framework NWChem and NWChemEx and exascale computing (Richard et al.)
- rOpenSci and best practices for developing software to support reproducible science (Ram et al.)
- Balancing reusable scientific software development with obtaining rapid scientific results (Adorf et al.)

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Community-led Culture Change in Research Software

- **Software Sustainability Institute (SSI):** Cultivating better and more sustainable research software to enable world-class research for the U.K. research community.
- **Conceptualization of a U.S. Research Software Sustainability Institute (URSSI):** Planning an institute to improve science and engineering research by supporting the development and sustainability of research software in the U.S.
- **IDEAS Productivity Project:** Catalyzing advances in software productivity and sustainability that are driven by the needs of extreme-scale computational science.
- **Better Scientific Software (BSSw):** Encouraging the exchange of information on practices, techniques, experiences, and tools to improve developer productivity and software sustainability for CSE and related areas of technical computing.

Community-led Culture Change in Research Software

- **Apache Software Foundation:** Fostering the growth of open-source software communities and providing the necessary technical infrastructure and support mechanisms.
- **Software Carpentry:** Teaching foundational coding skills to researchers and empowering them to develop research software, automate research tasks and workflows, and perform reproducible science.
- **Working Towards Sustainable Software for Science: Practice and Experiences (WSSSPE):** Promoting sustainable research software by addressing challenges related to the full lifecycle of such software via shared learning and community action.
- **NumFOCUS:** Promoting open code for better science while emphasizing sustainable high-level programming languages, open code development, and reproducible scientific research.

Community-led Culture Change in Research Software

- **rOpenSci**: Enabling open and reproducible research by creating technical and social infrastructure and advocating for a culture of data sharing and reusable software.
- **xSDK**: Promoting collaboration and commitment to independent numerical library efforts through community-based policies for quality improvement, better infrastructure, and the use of diverse libraries for large-scale CSE.
- **Research Software Alliance (ReSA)**: Bringing communities together to collaborate on the advancement of research software.

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