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Editorial: Scientific workflows at extreme scales

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Editorial on the Research Topic
Scientific workflows at extreme scales

Scientific computing is undergoing a transformation, driven by the growing availability of exascale platforms and the expanding complexity of scientific workflows. While exascale systems offer unprecedented opportunities for discovery, they also bring significant challenges. These include managing heterogeneous workloads, achieving efficient resource utilization, and integrating diverse computational components—from simulation and data analysis to machine learning—within a unified workflow. The Research Topic *Scientific Workflows at Extreme Scales* in *Frontiers in High Performance Computing* addresses these pressing concerns by presenting contributions that reflect not only innovations in algorithms and performance engineering but also holistic thinking about workflow design, coordination, and usability. For general information on computational workflows readers are referred to survey papers (Diercks, 2023) and (Silva et al., 2021).

A recurring theme across the papers in this Research Topic is the orchestration of complex, heterogeneous workflows that span facilities, software stacks, and disciplines. In *ExaFEL*, Blaschke et al. detail a 7-year cross-facility collaboration enabling real-time data processing for X-ray Free Electron Laser science, offering a blueprint for DOE's Integrated Research Infrastructure program. Similarly, Callaghan et al. describe the CyberShake platform, a multidisciplinary workflow producing seismic hazard models by orchestrating over 32,000 jobs and managing petabytes of data across advanced computing infrastructures. Both contributions highlight the growing importance of workflow tools capable of handling sustained, high-throughput computational campaigns.

Another critical focus of this Research Topic is on multiphysics and multiscale coupling. Trebotich et al. present a new framework for simulating subsurface fracture evolution, combining pore-scale flow and reactive transport with geomechanics through a custom data-coupling and geometry-tracking strategy. Watson et al. explore neutron scattering workflows, integrating domain-specific codes with exascale compute resources to extract scientific insight from increasingly complex data. Meanwhile, Min et al. assess performance portability and optimization of the thermal-fluids code NekRS across multiple GPU architectures, emphasizing the infrastructure-level considerations required to sustain production-level performance.

Finally, the ExaWorks SDK described by Turilli et al. showcases a proactive approach to building a sustainable software ecosystem for exascale workflows. By curating and integrating workflow technologies and emphasizing testability, documentation, and interoperability, this effort outlines best practices essential for enabling diverse scientific use cases on modern HPC systems.

Together, these contributions emphasize that scientific workflows are more than the sum of their computational parts—they are living systems, shaped by disciplinary needs, software engineering practices, and computing architectures. As we continue to push the boundaries of scientific discovery, workflow design and execution will remain central to our ability to harness exascale computing effectively and inclusively. We hope this Research Topic provides valuable insights, practical strategies, and inspiration for researchers navigating the rapidly evolving landscape of extreme-scale science.

Author contributions

AD: Writing – original draft. ED: Writing – review & editing.

Conflict of interest

The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

Generative AI statement

The author(s) declare that Gen AI was used in the creation of this manuscript. The authors used an AI tool to generate summaries of all the accepted papers.

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