Perspectives on Teamwork and AI in Scientific Computing

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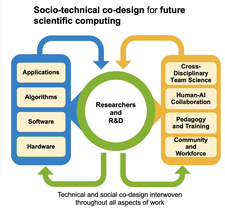
Next-Generation Ecosystems for Scientific Computing

Project Overview

Multi-Pronged Approach: Contribute to knowledge in ecosystems for scientific computing and help shape future developments across the DOE lab system and beyond through research on teams and AI and engagement with stakeholders across scientific computing community.



Socio-Technical Co-Design

- Intentional, integrated development of social and technical components as interdependent parts of a unified strategy.
- Integrate cutting-edge advances in AI and software (e.g., large language models (LLMs), scientific machine learning (SciML), reasoning models, coding agents) with strategies to foster cross-disciplinary team building, training, and collaboration.

Teams Research

Objective: Assess state of collaboration in scientific computing, emphasis on cross-disciplinary requirements and emerging AI technologies.

- Understanding how teams collaborate, learn, and adapt in the age of AI.
- Identifying factors that influence likelihood of success in cross-disciplinary collaboration.
- Elucidating opportunities to advance better collaboration, software, and science.

Methods

Systematic Literature Review
N = 27

Mixed Methods Survey
N = 79

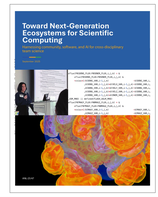
Semi Structured Interviews
N = 14

Community Engagement

Workshop Series: Convene experts in HPC, AI, computational science, applied mathematics, computer science, research software engineering, cognitive and social sciences, and community development to share, develop, and evaluate strategies for next-generation ecosystems in scientific computing.

Broad Engagement: Birds-of-a-feather Gathering at Trillion Parameter Consortium

Presentations and Publications



Teamwork is widely viewed as important across a range of priorities.

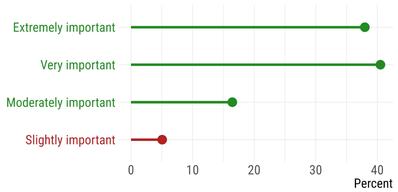


Figure 1. Responses to "Considering other priorities that you may have, how important is good teamwork in scientific computing for you?"

50% of those surveyed report relatively low to no awareness of best practices for teamwork.

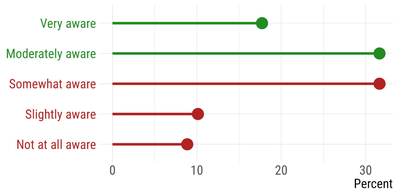


Figure 2. Responses to "Are you aware of any existing best practices for effective teamwork in scientific computing?"

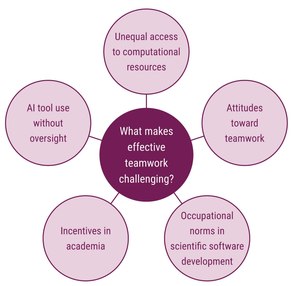


Figure 3. Challenges identified by study participants.

Only 14% of those surveyed report no AI use.

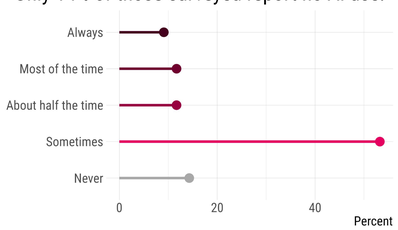


Figure 4. Responses to "Do you use AI in your work?"

56% of those surveyed report no team discussion on policy for AI use.

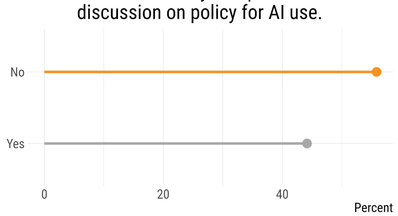


Figure 5. Responses to "Has your team considered formulating policies on the use of AI in your work?"

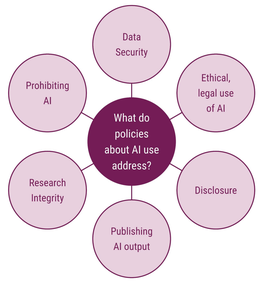


Figure 6. Policy topics reported by study participants.

Characterizing Teamwork in Scientific Computing

- Team formation driven by common goals, mutually beneficial outcomes, student work, conferences, shared affiliation, and prior collaborations [1-5].
- Multiteam systems, multiple team membership, and team boundary blurring are increasingly common.
  - Team interactions center on accessing and integrating expertise.
- Trust is a critical lever for expertise utilization and team viability in these cross-disciplinary teams.
  - *Competence-based trust*: "expectation that [teammate] has technical skills, experience, reliability needed to fulfill obligations" [6].
  - *Epistemic trust*: "trust in communication or communicated knowledge" [7].
- Participants report interest in training for communication, conflict management, and perspective taking.
- Participants identify visionary leaders, deep technical experts, project managers, and process experts as essential for team effectiveness.

How should we design workflows and tools for teams whose boundaries are shifting?

What training/resources do you wish you had for collaborating across disciplines?

What strategies can help cross-disciplinary teams bridge deep expertise gaps?

Determining the Role of Generative AI in Scientific Computing

- GenAI is generally seen as adequate for basic, minimal risk tasks (e.g., text editing, text summarization, well-defined problems).
- Participants describe opportunities for AI across software development lifecycle: writing, reviewing, testing, refactoring, and translating code.
  - Some see AI as increasing productivity while others see it as creating bloat, slop that increases workload.
- Reported best possible use for AI reflects perceived trustworthiness and competence of AI alongside attitudes toward and beliefs about AI.
  - Optimistic perspective: any role or task is reasonable as "*[AI] can support, basically, all roles, but it would always need supervision.*"
  - Pessimistic perspective: no role or task is acceptable as "*AI is a destroyer of reasoning, collaboration, [and] scientific insight*."
  - Ultimately, AI is often still viewed as a tool, and not a teammate.
- Participants identify a subset of roles and tasks as inappropriate or problematic for AI: leadership, project management, and community outreach.
- Participants caution against fully AI-generated computing systems, as these risk eroding human understanding and judgment.

What's in your team's AI policy? What should be added to or removed from the policy?

What training would help you leverage AI in your work?

What strategies are needed for trustworthy AI-enabled scientific computing?

Connecting AI and Teamwork in Scientific Computing

- Participants report that they do not perceive a direct effect of AI on teamwork.
  - Why? AI is not designed for teams, and it is often used independently by individual team members.
  - But, AI use is altering task processes and output at individual and team level, and some participant responses indicate AI use is affecting team dynamics due to differences between AI output and team member expertise.
  - Shared mental models about project task and technologies, including AI, are important. These models weaken when teams do not discuss AI use.
- Our results highlight promises and pitfalls for leveraging and augmenting expertise with AI in teams. For example:
  - Participants envision opportunities for accelerated access and development of expertise with AI, particularly among junior scholars and early career researchers, such that AI can be utilized for "easy" questions and team interactions focus on project vision and complex problems.
  - "*Scientific computing is often an individual experience*": Participants report that they experience isolation working in scientific computing and have limited opportunities to build familiarity and engage in meaningful teamwork episodes. Reliance on AI may exacerbate these conditions.

How do you feel about AI as teammate? Can/should AI be a fully-fledged teammate?

How do we leverage AI for science without diminishing the value of teamwork?

How do we design AI for cross-disciplinary teamwork?

Future Directions: (1) Share the full results of our research via a publication, and (2) develop open training materials and resources tailored to the needs of scientific software teams.

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Study Methods and Poster References

Workshop Series Year 1 Report