ASCR and Community Research Priorities

Focusing on Relevance to Compiler Technology

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The Mission of the Department of Energy

The mission of the Energy Department is

to ensure America's security and prosperity

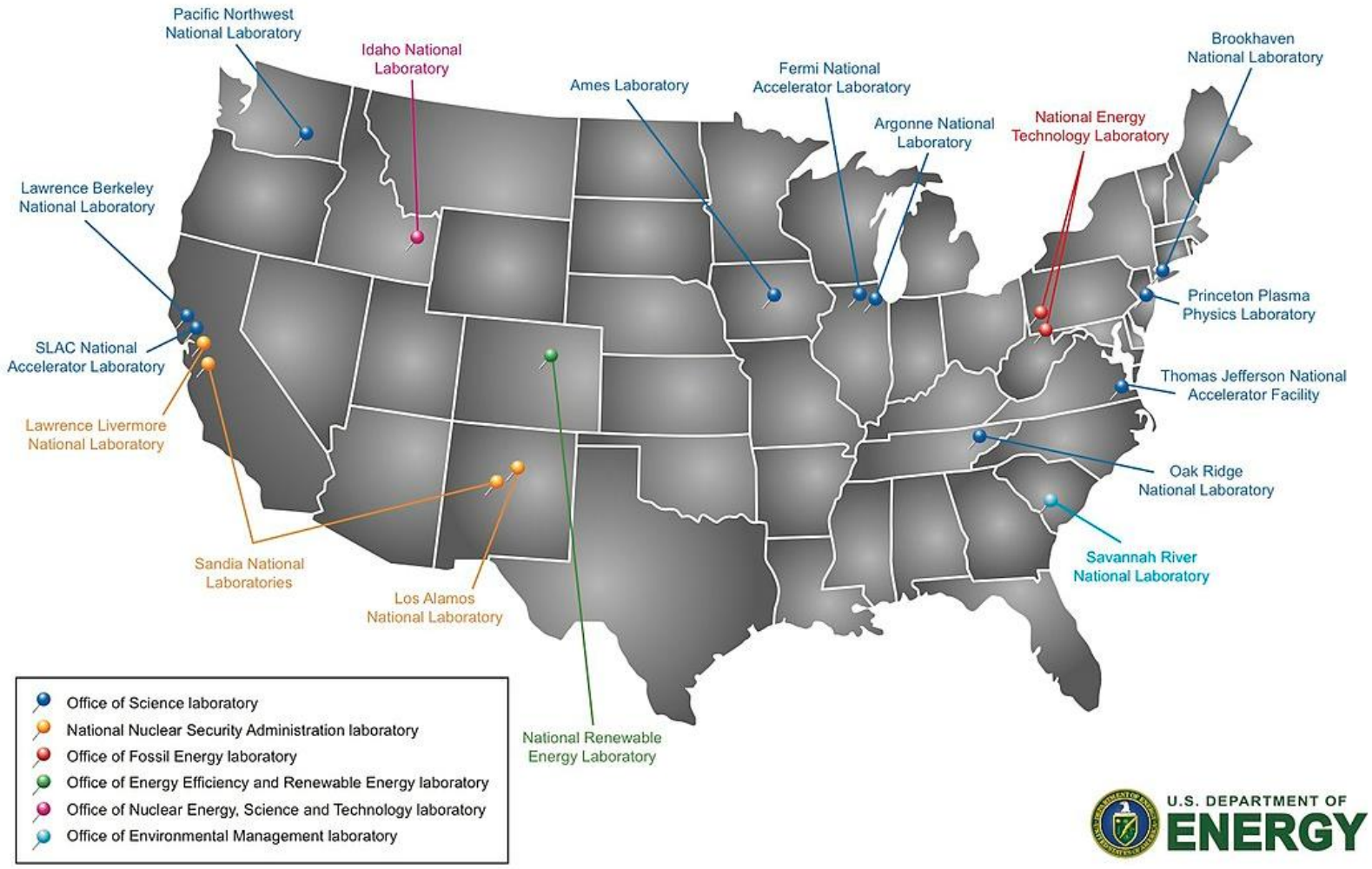
by addressing its energy, environmental, and nuclear challenges

through transformative science and technology solutions.

DOE Science Programs

Basic Energy Sciences	• Understanding, predicting, and ultimately controlling matter and energy flow at the electronic, atomic, and molecular levels
Advanced Scientific Computing Research	• Advancing state-of-the-art computational, networking, data, and software capabilities that enable scientific discovery
Biological and Environmental Research	• Understanding complex biological, climatic, and environmental systems
Fusion Energy Sciences	• Building the scientific foundations for a fusion energy source
High Energy Physics	• Understanding how the universe works at its most fundamental level
Nuclear Physics	• Discovering, exploring, and understanding all forms of nuclear matter

DOE National Laboratories



https://www.energy.gov/maps/doe-national-laboratories

ASCR Program Structure

US Department of Energy (DOE), Office of Science (SC), Advanced Scientific Computing Research (ASCR)
https://science.osti.gov/ascr

Facilities Division
National user facilities: ALCF, OLCF, NERSC, ESNet

Computational-Science Research and Partnerships Division

Advanced Computing Technologies (ACT) Division

Computational Partnerships

Computer Science

Applied Mathematics

For more information, see our FY23 budget request.

ASCR R&D Funding

Funding Opportunity Announcements (FOAs)

- https://science.osti.gov/ascr/Funding-Opportunities
- Announced on grants.gov (hint: sign up for email notifications for 'ASCR')
- Read each announcement carefully to understand who can apply and other restrictions/requirements
- Depending on the announcement, supports 2–5-year projects
- University researchers can apply directly (please coordinate with your organization's sponsored-research office)
- Subcontracting is often permitted, and sometimes collaborative applications are permitted

Early Career Research Program

- https://science.osti.gov/early-career
- Research grants for five years
- Stays with PI if PI changes institutions
- Eligible within 10 years of Ph.D. (can apply up to three times)
- University-based researchers receive about $150,000/year
- Topics released in the summer, pre-applications generally due in the fall

DOE National Laboratory Announcements

- https://science.osti.gov/ascr/Funding-Opportunities (bottom of the page)
- Open only to DOE Laboratories
- Often allow subcontracts to support collaborators at other organizations

Small Business Innovation Research (SBIR) and Small Business Technology Transfer (STTR)

- https://science.osti.gov/sbir
- Grants to for-profit US businesses with 500 or fewer employees (including affiliates)
- Phase I: ~$200k for 6-12 months, Phase II: ~$1M for 2 years
- Subcontracting is permitted, STTR: requires collaboration with a research Institution
- Topics released in the summer, pre-applications generally due in the fall

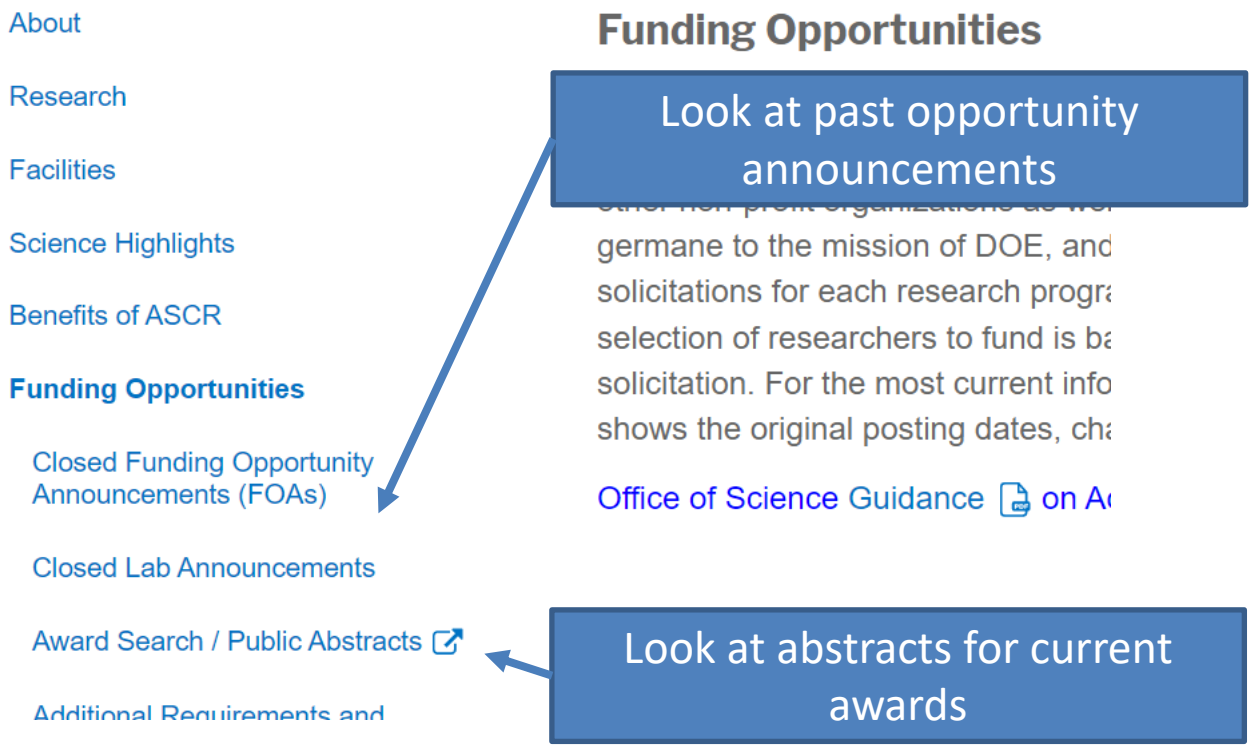
Computational Science Graduate Fellowship (CSGF)

http://www.krellinst.org/csgf/

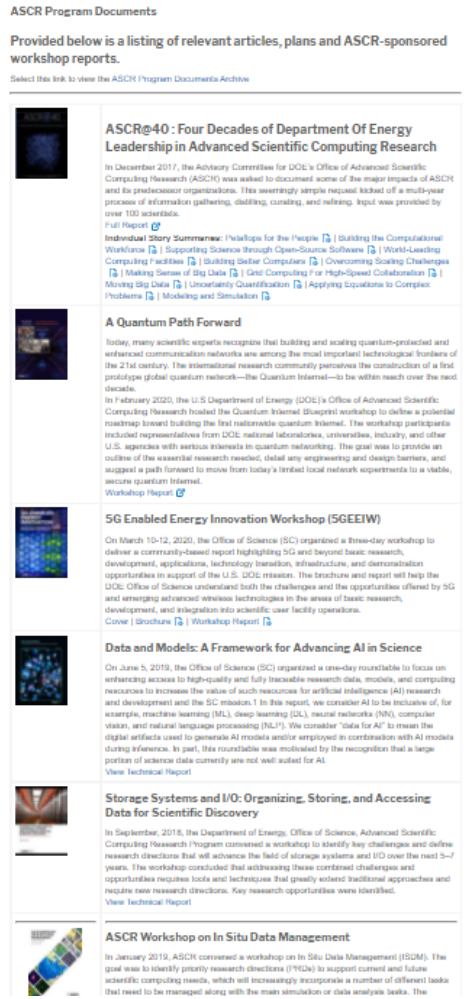
Additional Information on ASCR's Website

https://science.osti.gov/ascr/Funding-Opportunities

https://science.osti.gov/ascr/Community-Resources/Program-Documents



Look at recent reports from ASCR-sponsored workshops. These discuss priority research directions, as identified by the research community, along with relevant background information, in various areas.



https://www.orau.gov/ASCR-CoDesign/

232 Registered Attendees
- 86 Observers
- 146 Participants
  - 110 - Laboratory Staff
  - 18 - University Faculty/Staff
  - 13 - Industry (including AMD, ARM, GE, Google, Intel, Micron, NVIDIA, Qualcomm, Xilinx)
  - 5 - Other Federal Agencies

ASCR Point of Contact: Hal Finkel

ASCR Workshop on Reimagining Codesign: Videos

https://www.orau.gov/ASCR-CoDesign/

Keynotes were provided by:

- Neil Thompson, MIT
- Margaret Martonosi, Princeton/NSF
- Andreas Olofsson, Zero ASIC

Organizing Committee:

John Shalf, LBL

Andrew A Chien, ANL

Jeff Vetter, ORNL

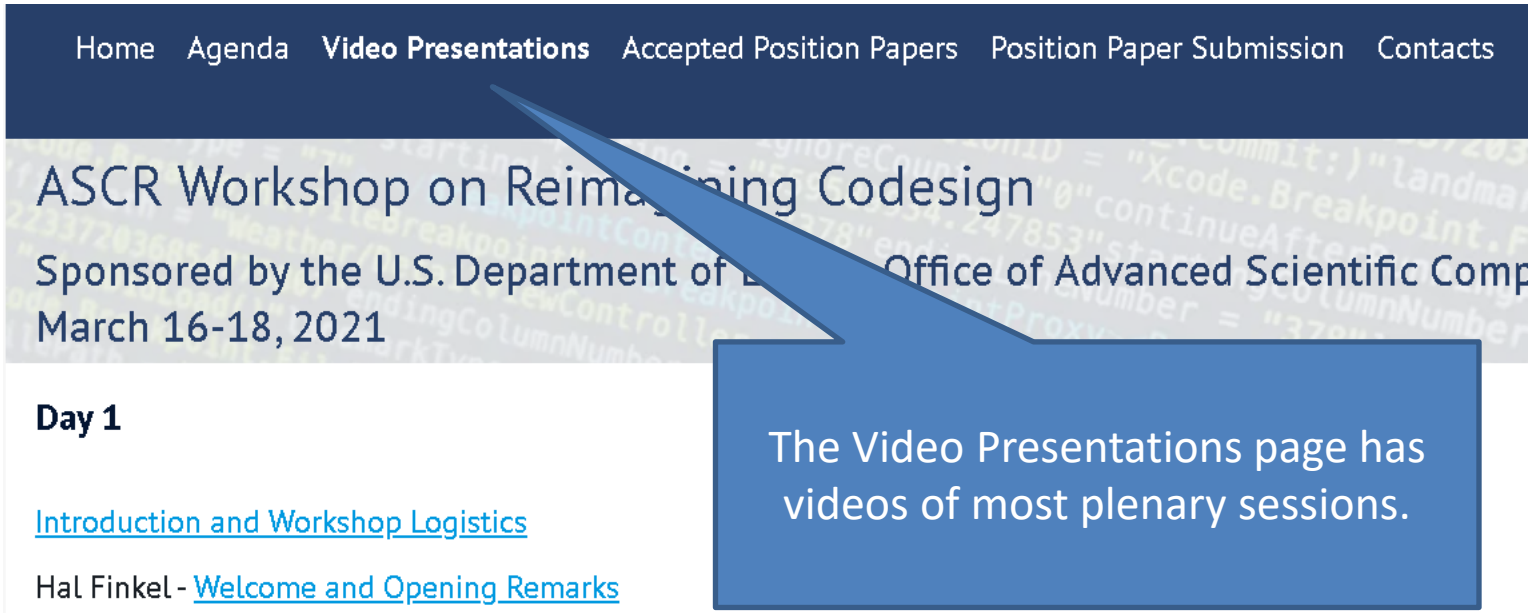
Jim Ang, PNNL

Adolfy Hoisie, BNL

Si Hammond, SNL

Ian Karlin, LLNL

Scott Pakin, LANL



The Video Presentations page has videos of most plenary sessions.

ASCR Workshop on Reimagining Codesign: Position Papers

https://www.orau.gov/ASCR-CoDesign/

- A general call for position papers was issued.
- The organizing committee reviewed the papers.
- One author of each accepted paper was invited to participate in the workshop.
- Collection of accepted position papers: https://doi.org/10.2172/1843574

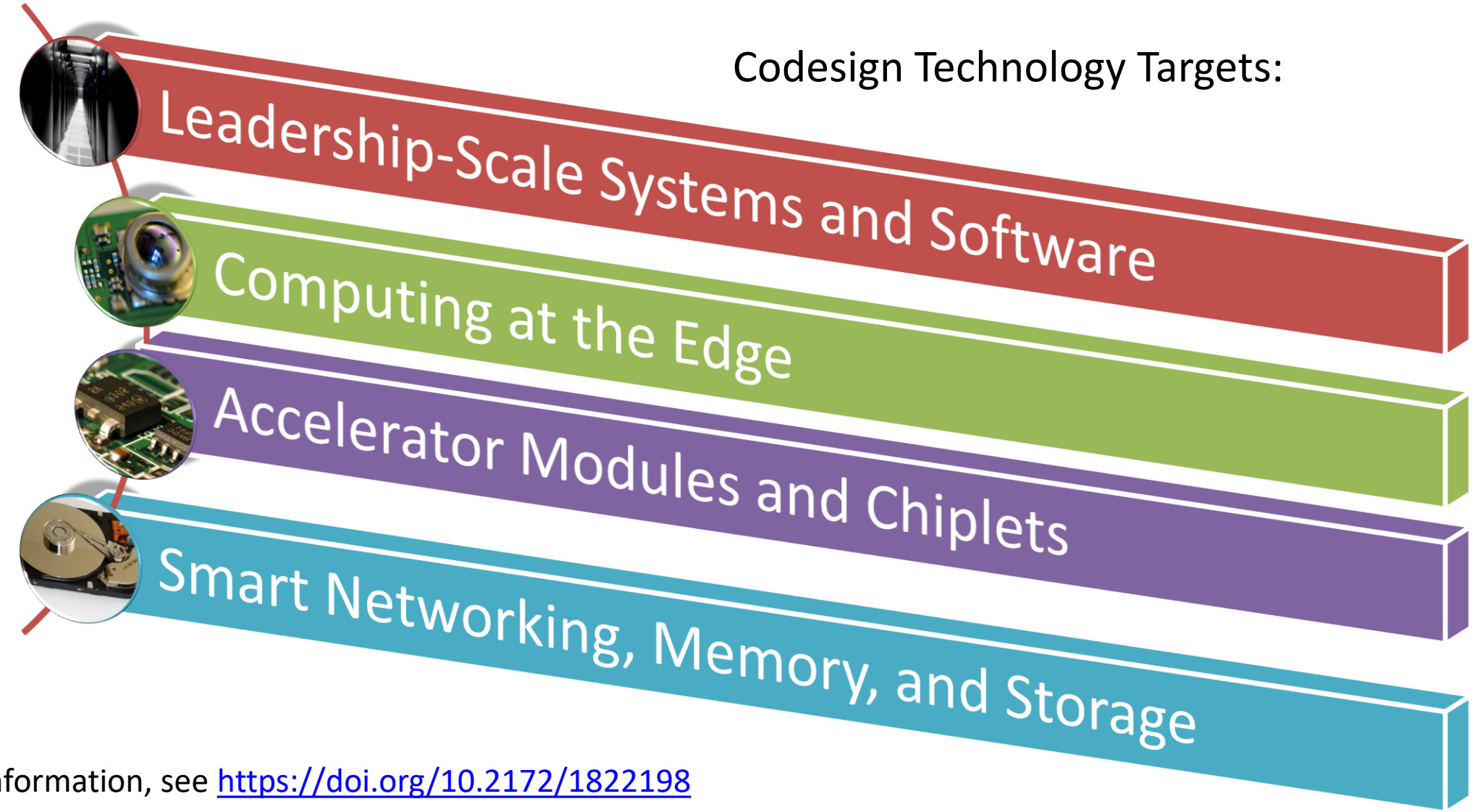
The Accepted Position Papers page has the 86 accepted position papers.

Author	Institutional Affiliation	
Alex Aiken	Stanford/SLAC	Codesign
Tim Ansell	Google	Missing pieces for accelerating co-design to meet the growing Moore's Law
Richard Arthur	GE Research	An (Evolving) Rubric for Modeling Maturity
Amro Awad	North Carolina State University	Codesign for Disaggregated Memory Architectures: Opportuni
Amro Awad	North Carolina State University	Microarchitecture-Centric Codesign for Reduced TCO and High
Abdel-Hameed Badawy	New Mexico State University	Utilizing Recent Advances in NLP-ML for HW/SW Codesign
Prasanna Balaprakash	Argonne National Laboratory	An AI System for AI Codesign
Kevin Barker	Pacific Northwest National Lab	Advanced Architecture Assessment Within a Codesign Metho

ASCR Workshop on Reimagining Codesign: Technology Targets

https://www.orau.gov/ASCR-CoDesign/

Codesign Technology Targets:

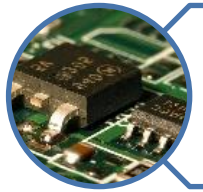


For more information, see https://doi.org/10.2172/1822198

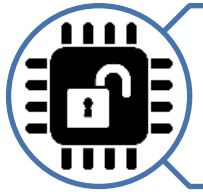
ASCR Workshop on Reimagining Codesign: Enabling Technology Factors

https://www.orau.gov/ASCR-CoDesign/

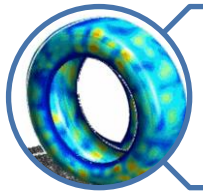
Enabling Key Technology Factors:



Advanced, modular packaging technologies providing for the high-performance composition of components optimized for different computational motifs, potentially from different organizations



Open-source hardware designs allowing open, low-risk collaboration among academics, laboratories, and industry



AI-driven technologies, paired with advanced system modeling, creating intelligent, data-driven workflows for hardware design and software development

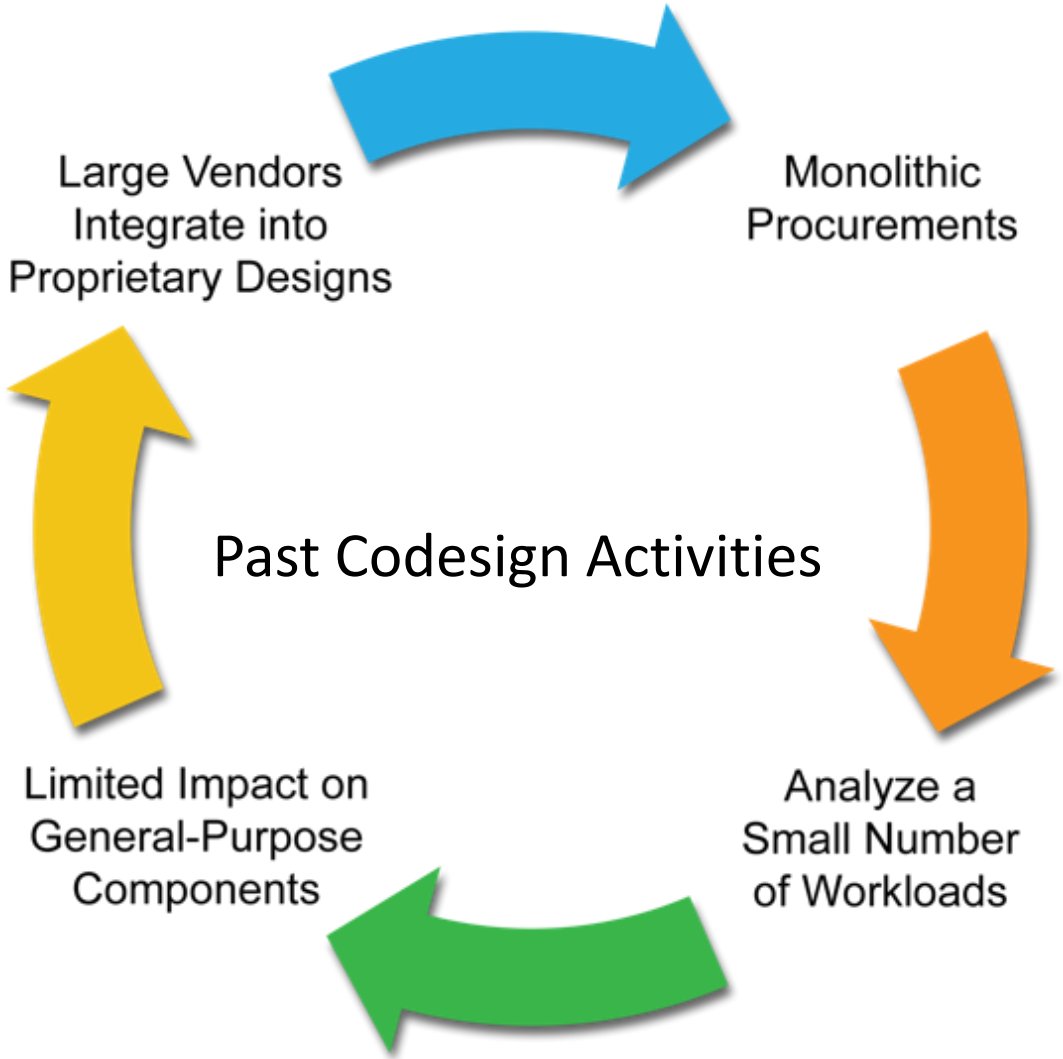
Critical metrics for energy efficiency, security, and other system properties have joined performance, power usage, and reliability as first-class design constraints

The foundations laid in pursuit of exascale computing have generated applications capable of using first-generation heterogeneous GPU computing resources through **portable programming models and adaptive system software**

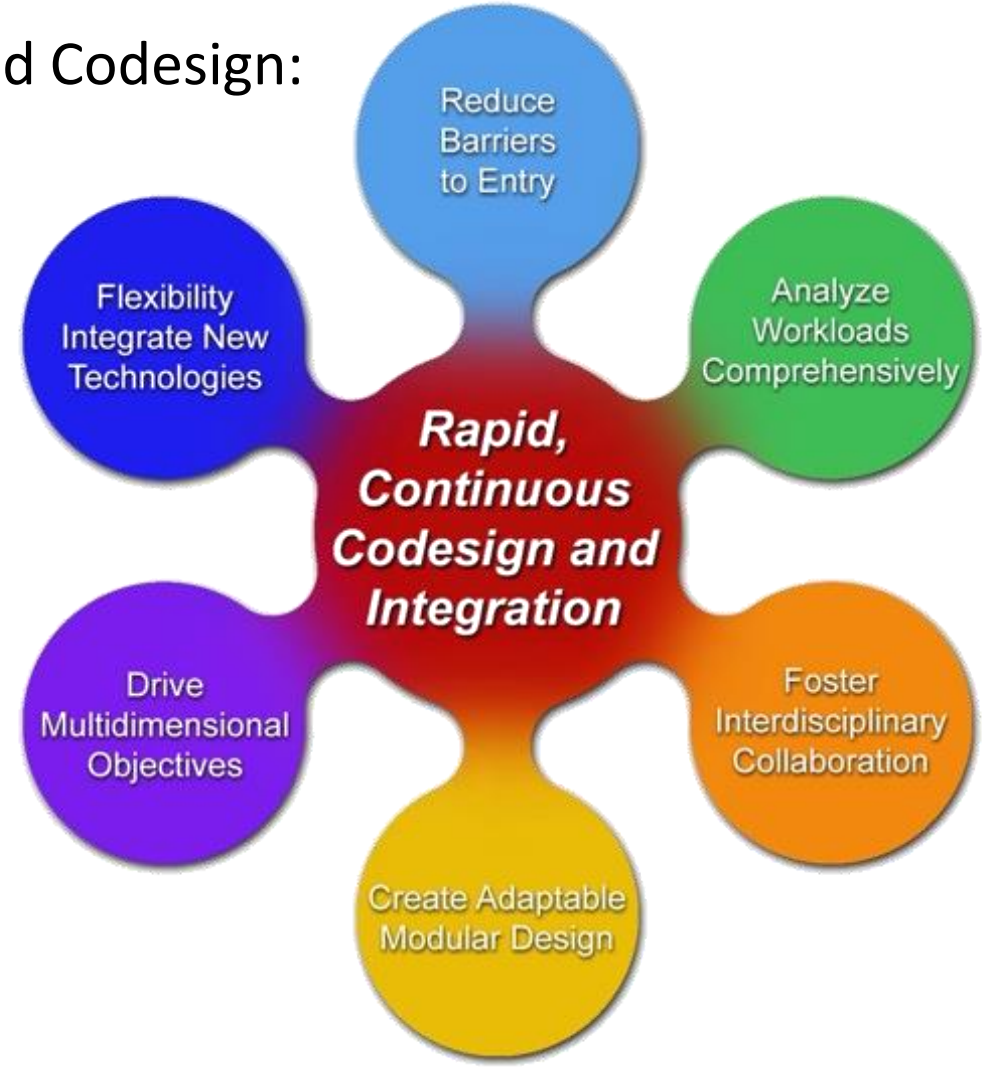
For more information, see https://doi.org/10.2172/1822198

ASCR Workshop on Reimagining Codesign: Past vs. Future

https://www.orau.gov/ASCR-CoDesign/



Reimagined Codesign:



For more information, see https://doi.org/10.2172/1822198

Priority Research Directions:

1. Drive Breakthrough Computing Capabilities with Targeted Heterogeneity and Rapid Design

Key Questions: What new methods and technologies are required to rapidly create breakthrough hardware designs? How can we ensure that they align to support increasingly diverse and demanding computing requirements?

2. Software and Applications that Embrace Radical Architecture Diversity

Key Question: What novel approaches to software design and implementation can be developed to provide performance portability for applications across radically diverse computing architectures?

3. Engineered Security and Integrity from Transistors to Applications

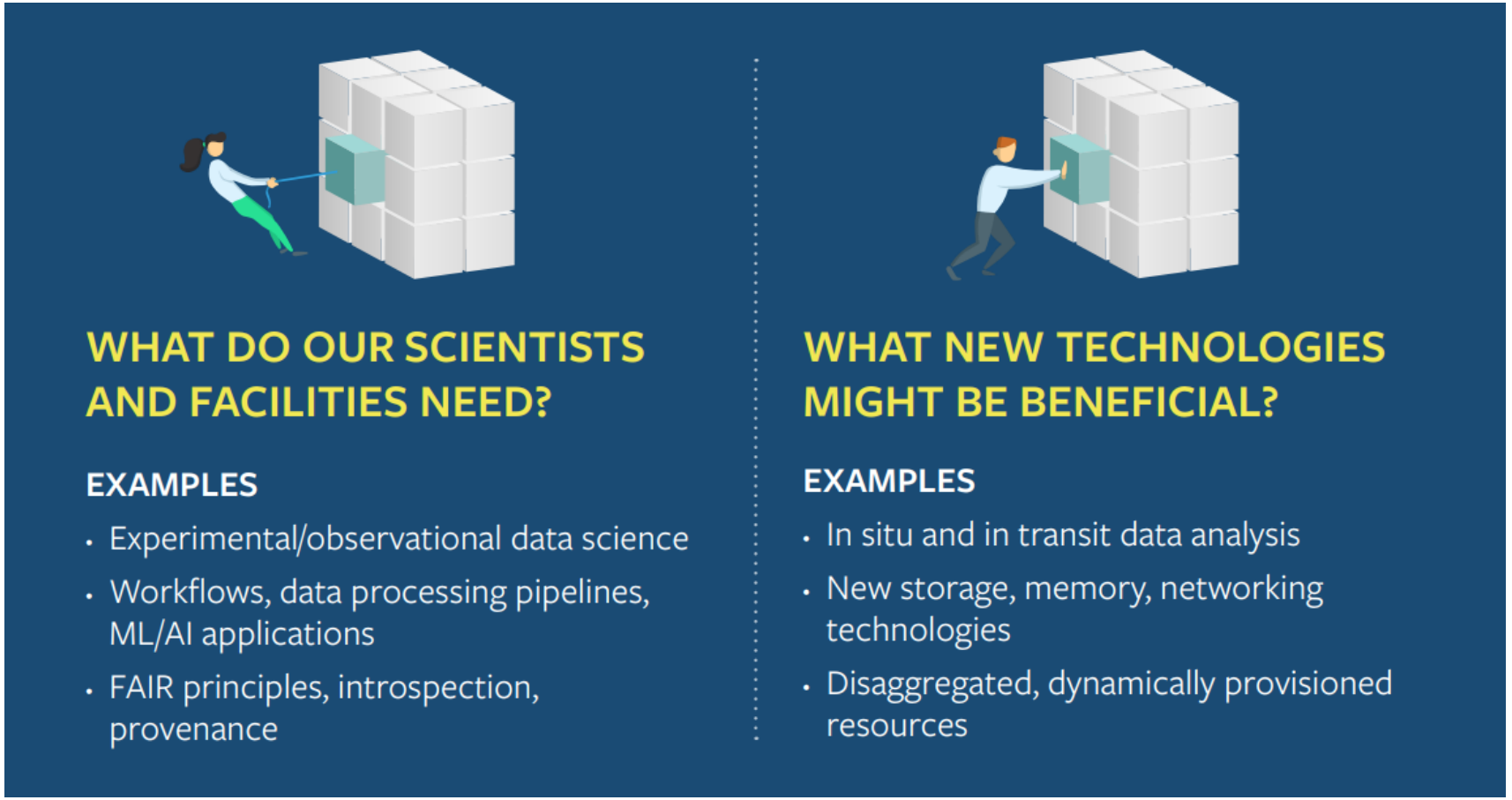
Key Questions: How does codesign consider needs for end-to-end scientific computing and scientific data security, provenance, integrity, and privacy? What computer security innovations from the commercial computing ecosystem (e.g., trusted execution environments) can be codesigned to provide security for DOE scientific discovery? How do we validate components with increasingly diverse supply chains and sources of development?

4. Design with Data-Rich Processes

Key Questions: What are the quantitative tools that are practical, accurate, and applicable to codesigning various layers of the hardware/software stack and of data-driven, dynamic, irregular workflows, such as those occurring in experimental science or AI/machine learning workloads?

For more information see https://doi.org/10.2172/1822198. The workshop report will be available from https://doi.org/10.2172/1822199 upon publication.

ASCR Workshop: The Management and Storage of Scientific Data



https://www.osti.gov/biblio/1845705-management-storage-scientific-data

ASCR Workshop: The Management and Storage of Scientific Data

1. High-productivity interfaces for accessing scientific data efficiently

Key Questions:

1. How can application developers search and access important information seamlessly in massive amounts of scientific data?
2. What changes are needed to existing I/O application programming interfaces (APIs) to enable complex AI workflows?
3. What are effective interfaces and abstractions for capturing user intent for optimizing data management?

2. Understanding the behavior of complex data management systems in DOE science

Key Questions:

1. How can disparate information from multiple sources regarding data management activities be fused into useful knowledge?
2. In what ways can people and software leverage this knowledge to improve the reliability and performance of data management systems?

https://www.osti.gov/biblio/1845705-management-storage-scientific-data

ASCR Workshop: The Management and Storage of Scientific Data

3. Rich metadata and provenance collection, management, search, and access

Key Questions:

1. What metadata and provenance are needed to support FAIR principles?
2. How do we support collection, storage, and search of rich metadata and provenance?
3. How can we use rich metadata and provenance for optimizing data management?

4. Reinventing data services for new applications, devices, and architectures

Key Questions:

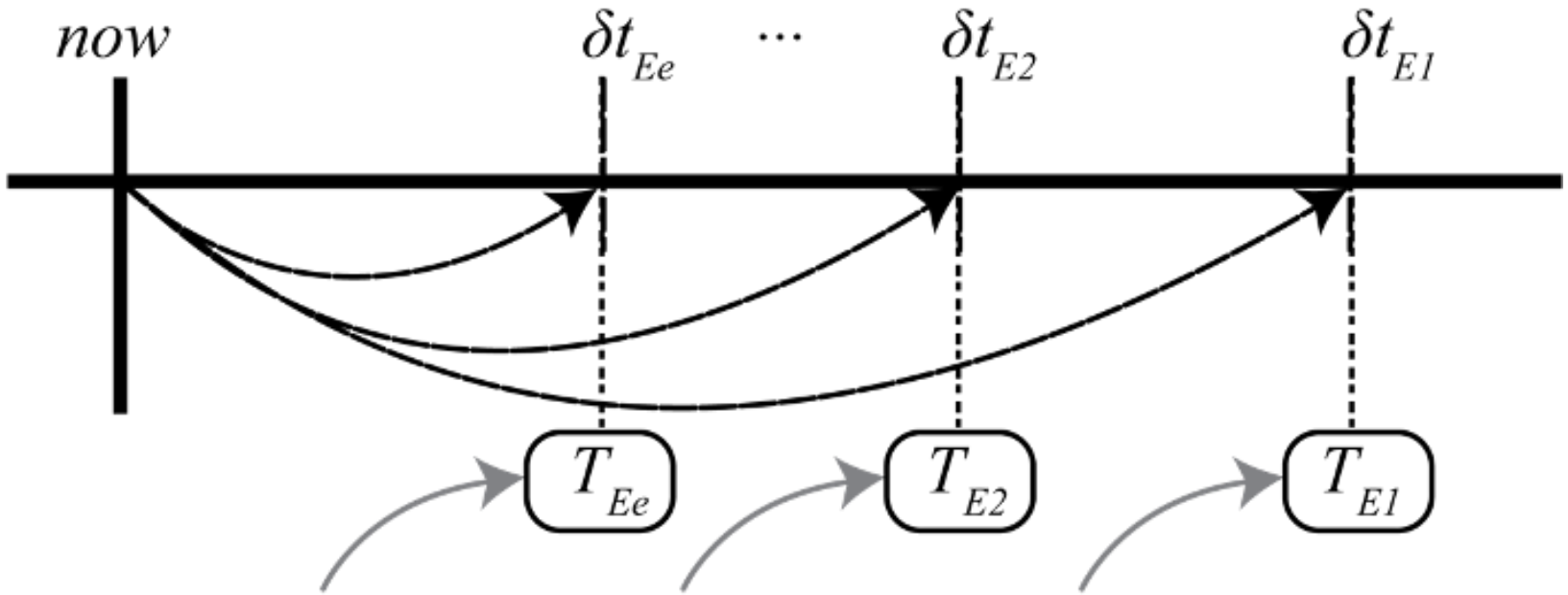
1. Using a co-design approach, how do we create specialized data services leveraging emerging device technologies to enable revolutionary breakthroughs across the breadth of DOE science?

https://www.osti.gov/biblio/1845705-management-storage-scientific-data

ASCR Roundtable on Parallel Discrete Event Simulation (PDES)

- September 20, 2021. 12-5pm Eastern Time.
- 21 participants from 8 labs (ANL, BNL, LANL, LBL, LLNL, ORNL, PNNL, SNL).
- ASCR points of contact: Hal Finkel, Randall Laviolette

- Parallel Discrete Event Simulation (PDES): Simulations modeling systems characterized by discrete state changes of, and discrete interactions between, a distributed collection of entities.

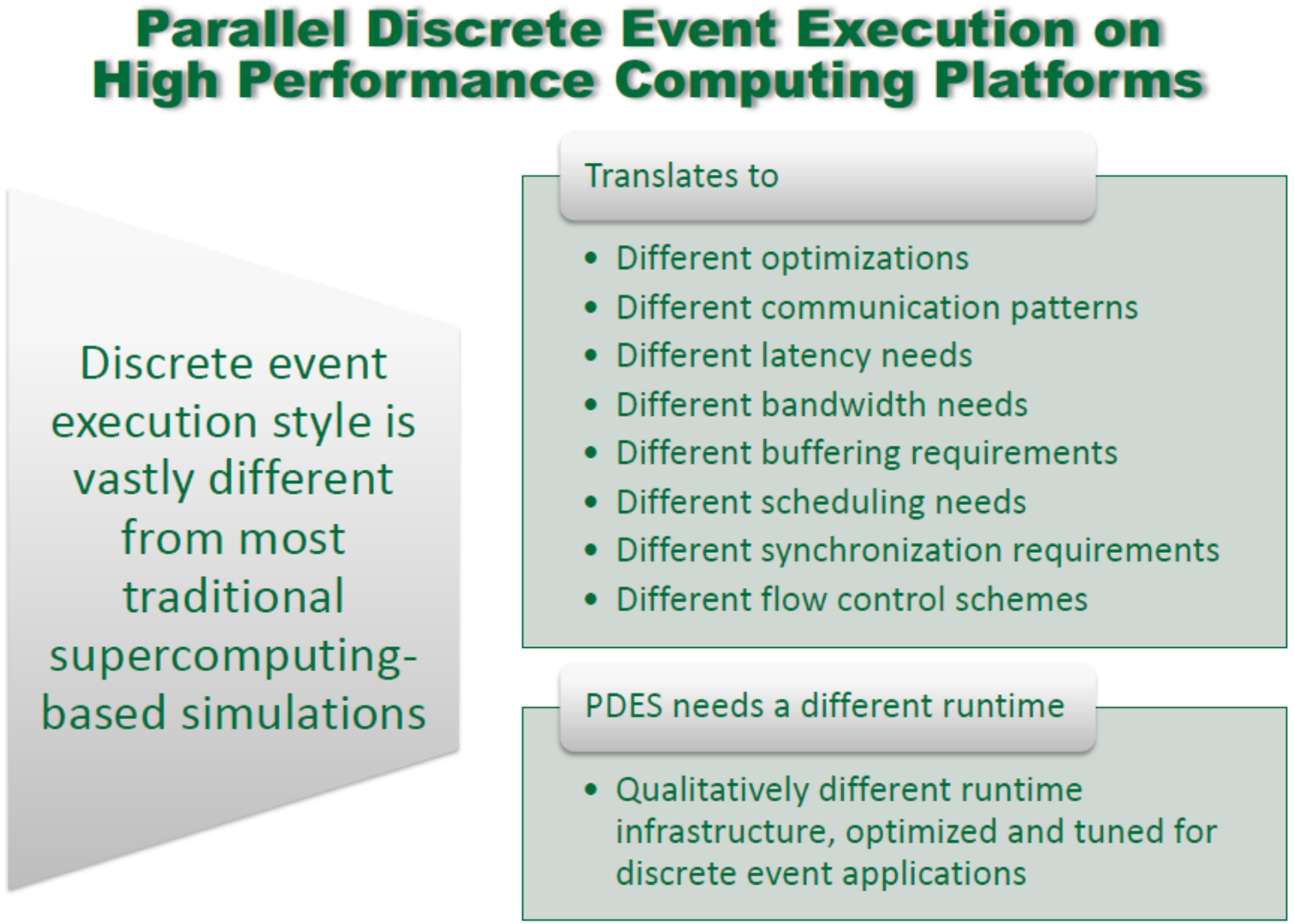


ASCR Roundtable on PDES: Use Cases

- Motivating use cases discussed included:
  - Transportation and Mobility Applications
    - A collection of distributed agents (e.g., vehicles and infrastructure controllers), each optimizing either their individual utility (e.g., user travel time) or system efficiency (e.g., minimize congestion or fuel).
    - Transportation systems are becoming increasingly complex and interconnected (e.g., real-time GPS and camera data feeds, 5G, and smart infrastructure and vehicles). [Also applies analogously below.]
  - Energy Grid Applications
    - Models distributed control systems for, and behavior of, smart grids and renewable energy grids.
  - Internet and Cybersecurity Simulations
    - Models networking infrastructure (hosts, routers, etc.) and protocols.
  - Material Science Applications using Kinetic Monte Carlo
    - Models many processes including crystal grain growth, thin film growth, dopant migration in semiconductors, and material evolution due to radiation damage.
  - Epidemiological Planning, Response, Policy, and Decision-making
    - Models collective societal behavior from individual stochastic decisions and coupled physical systems.
  - Simulations for Hardware Co-Design and Large-Scale Scientific Infrastructure
    - Models hardware and application behavior across many scales, from circuits to supercomputers.

PDES brings notable opportunities for hardware/software co-design.

Thus, both PDES for co-design and co-design for PDES are relevant for future research.

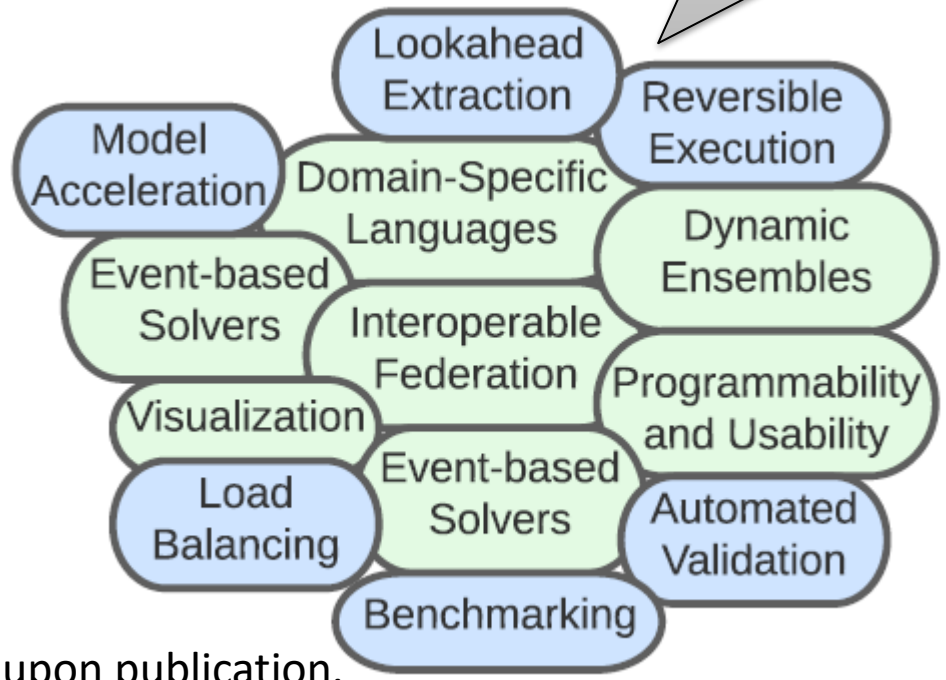


ASCR Roundtable on PDES: Research Opportunities

Research opportunities identified in:

- Core Advancements (Inner Technologies)
  - Exploiting supercomputing/accelerator architectures
  - Parallel decomposition, dynamic load balancing, and event scheduling
  - Incorporating AI/ML (as surrogates, for speculative execution, etc.)
- Usability Advancements (Outer Technologies)
  - Interoperable and federated execution
  - Adaptive ensembles
  - Visualization techniques
  - Use of streaming data
  - Interfaces and domain-specific languages (e.g., for lookahead extraction, reverse execution)
  - Runtime adaptation, event aggregation, and scheduling
- Advancements for the Scientific Enterprise and Mission Applications
- (Cross-cut Technologies)
  - Simulations of the DOE Science Enterprise
  - PDES-based Mathematical Solvers
  - Benchmarks and other domain-informed developments

Interestingly, compilation for reversible execution also comes up in work on energy-efficient and quantum computing.



The roundtable report will be available from https://doi.org/10.2172/1855247 upon publication.

Some Other Past ASCR Workshops and Roundtables

Roundtable Report: Terahertz and 6G Wireless Communications in Science and Extreme Environments

The main objective of the roundtable is to explore the potential of Terahertz (THz) and 6G communications in extreme environments such as industrial, manufacturing, and large critical scientific facilities (for example, light sources, accelerators, high-performance computers, data centers, neutron sources, etc.). In contrast to commercial wireless networks (5G included), which are optimized for best-effort broadband voice and Internet of Things (IoT) services.

Report October 1, 2020

5G Enabled Energy Innovation Workshop (5GEEIW)

On March 10-12, 2020, the Office of Science (SC) organized a three-day workshop to deliver a community-based report highlighting 5G and beyond basic research, development, applications, technology transition, infrastructure, and demonstration opportunities in support of the U.S. DOE mission. The brochure and report will help the DOE Office of Science understand both the challenges and the opportunities offered by 5G and emerging advanced wireless technologies in the areas of basic research, development, and integration into scientific user facility operations.

Cover | Brochure | Workshop Report

https://science.osti.gov/ascr/Community-Resources/Program-Documents

Some Other Past ASCR Workshops and Roundtables

Data and Models: A Framework for Advancing AI in Science

On June 5, 2019, the Office of Science (SC) organized a one-day roundtable to focus on enhancing access to high-quality and fully traceable research data, models, and computing resources to increase the value of such resources for artificial intelligence (AI) research and development and the SC mission.1 In this report, we consider AI to be inclusive of, for example, machine learning (ML), deep learning (DL), neural networks (NN), computer vision, and natural language processing (NLP). We consider "data for AI" to mean the digital artifacts used to generate AI models and/or employed in combination with AI models during inference. In part, this roundtable was motivated by the recognition that a large portion of science data currently are not well suited for AI.

View Technical Report

ASCR Workshop on In Situ Data Management

In January 2019, ASCR convened a workshop on In Situ Data Management (ISDM). The goal was to identify priority research directions (PRDs) to support current and future scientific computing needs, which will increasingly incorporate a number of different tasks that need to be managed along with the main simulation or data analysis tasks. The workshop identified six PRDs that highlight the components and capabilities needed for ISDM to facilitate scientific discovery from a variety of different data sources.

Cover | Brochure | Report

https://science.osti.gov/ascr/Community-Resources/Program-Documents

Some Other Past ASCR Workshops and Roundtables

Report on Basic Research Needs for Scientific Machine Learning: Core Technologies for Artificial Intelligence

Scientific Machine Learning (SciML) and Artificial Intelligence (AI) will have broad use and transformative effects across the Department of Energy. Accordingly, the ASCR January 2018 Basic Research Needs workshop report identifies six Priority Research Directions (PRDs) as viewed through the lens of applied mathematics and scientific computing. The six PRDs provide a sound basis for a coherent, long-term research and development strategy in SciML and AI.

Cover | Workshop Report | Brochure

STREAM2016: Streaming Requirements, Experience, Applications and Middleware Workshop

This report describes the discussions, outcomes, and conclusions from STREAM2016: Streaming Requirements, Experience, Applications and Middleware Workshop – the second workshop in the STREAM series, held on March 22-23, 2016 in Tysons, VA. STREAM2016 focused on DOE applications, computational and experimental facilities, as well as software systems. The role of streaming and steering as a critical aspect of the linkage between experimental and computing facilities was pervasive throughout the workshop. Given the overlap in interests and challenges faced by industry, the workshop had significant presence from several major companies in this area.

Workshop Report.

https://science.osti.gov/ascr/Community-Resources/Program-Documents

ASCR Software-Stewardship Request for Information (RFI)

- On October 29th, 2021, ASCR released an RFI on the stewardship of software for scientific and high-performance computing.
- Responses were due by December 13th, 2021.

- The RFI details the potential scope of stewardship activities, including but not limited to:
  - Training on software development and use
  - Workforce support
  - Infrastructure for common development needs
  - Curation and governance processes
  - Maintaining situational awareness
  - Shared engineering resources
  - Project support

- ASCR received 37 independent responses*, quality of most was very high
  - ECP responses from the ECP ST leadership team, the ECP task force on broader engagement, NWChemEx Project.
  - 11 responses from DOE national laboratories.
  - Responses from non-profit organizations: HDF5 Group and NumFOCUS.
  - Response from the US Research Software Engineer Association
  - 6 responses from small businesses.
  - Responses from medium/large businesses: CloudBees, HPE, NVIDIA, Google.
- Responses available: https://doi.org/10.2172/1843576 – over 360 pages of text were provided.

(*) Counting the two independently-authored submissions from SNL separately.

ASCR Software-Stewardship RFI: Summary

Note: The following slides summarize themes noted in the RFI responses, and they are ***not*** comprehensive. Their purpose is to inspire interest in reading the RFI responses, available at https://doi.org/10.2172/1843576. No endorsement, recommendation, or favoring is intended or implied.

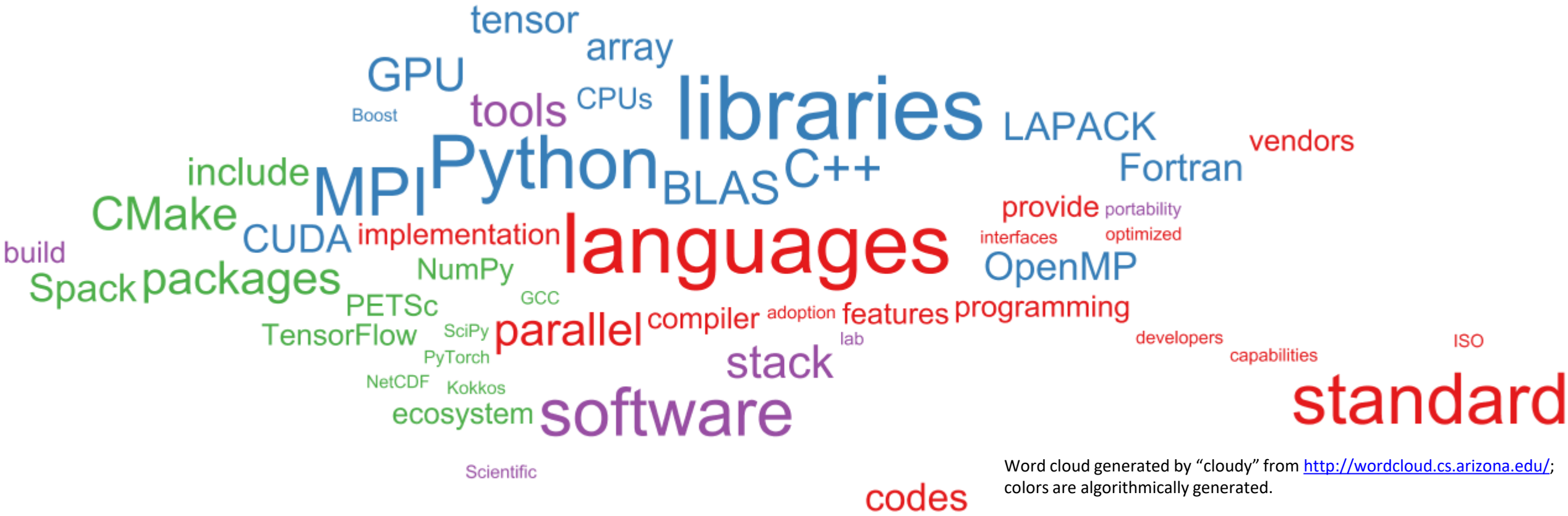
DOE thanks all of the respondents for their considerable collective effort and hopes that the RFI responses will serve as a resource for the entire community.

ASCR Software-Sustainability Task Force:
Ben Brown, Hal Finkel, Saswata Hier-Majumder, Robinson Pino, Bill Spotz

Note: For the full set of slides on the RFI responses, please see: https://science.osti.gov/-/media/ascr/ascac/pdf/meetings/202203/ASCAC_202203_Finkel-RFI-Codesign-PDES.pdf – This presentation contains only a subset of the slides.

ASCR Software-Stewardship RFI: Software Dependencies

Software dependencies and requirements: What software packages and standardized languages or Application Programming Interfaces (APIs) are current or likely future dependencies for your relevant research and development activities?

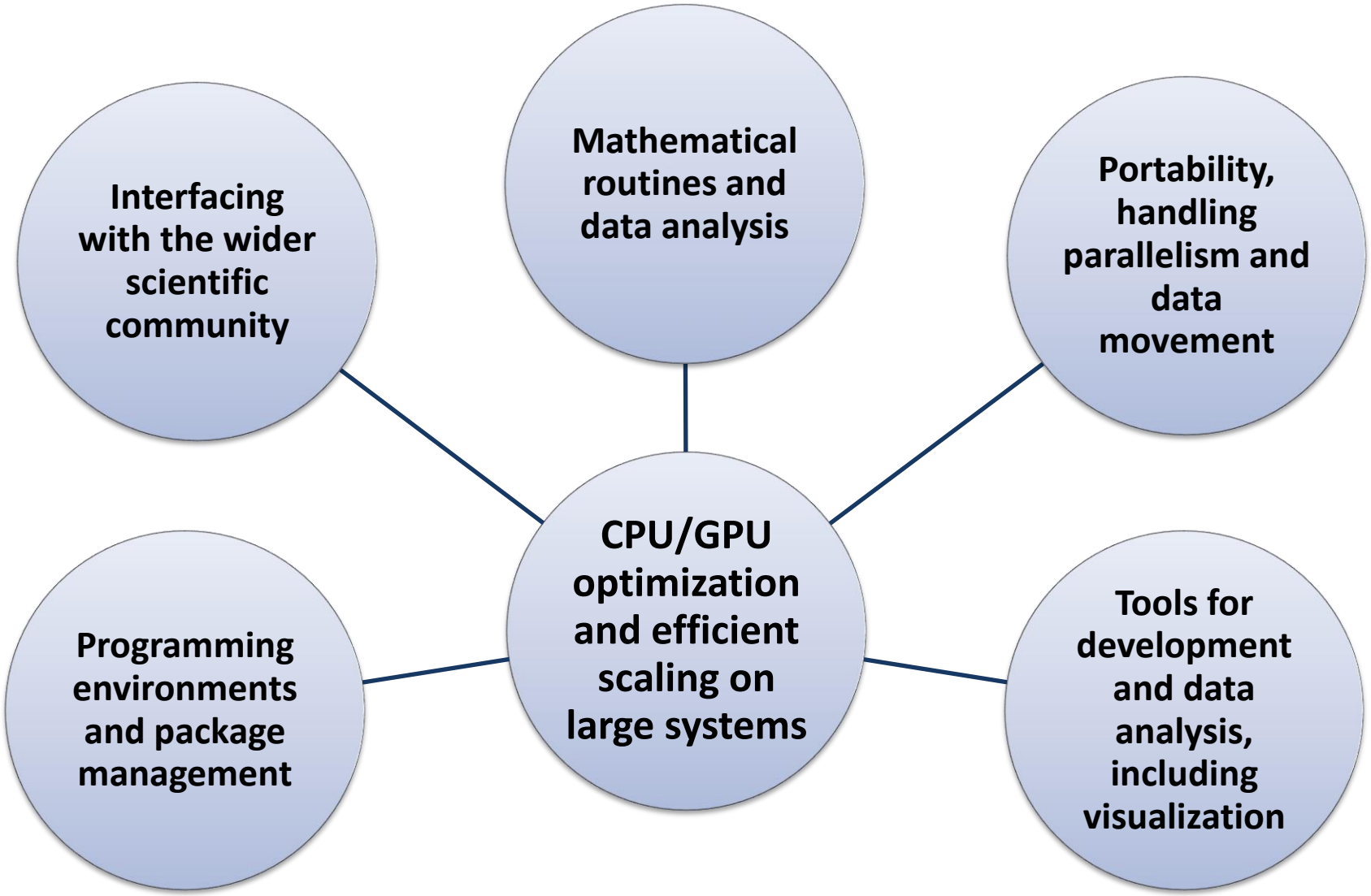


Word cloud generated by "cloudy" from http://wordcloud.cs.arizona.edu/; colors are algorithmically generated.

This slide summarizes themes noted in the RFI responses and is ***not*** comprehensive. No endorsement, recommendation, or favoring is intended or implied.

ASCR Software-Stewardship RFI: Key Capabilities Provided by Dependencies

Software dependencies and requirements: What key capabilities are provided by these software packages?



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ASCR Software-Stewardship RFI: Anticipated Key Capability Requirements

Software dependencies and requirements: What key capabilities, which are not already present, do you anticipate requiring within the foreseeable future?

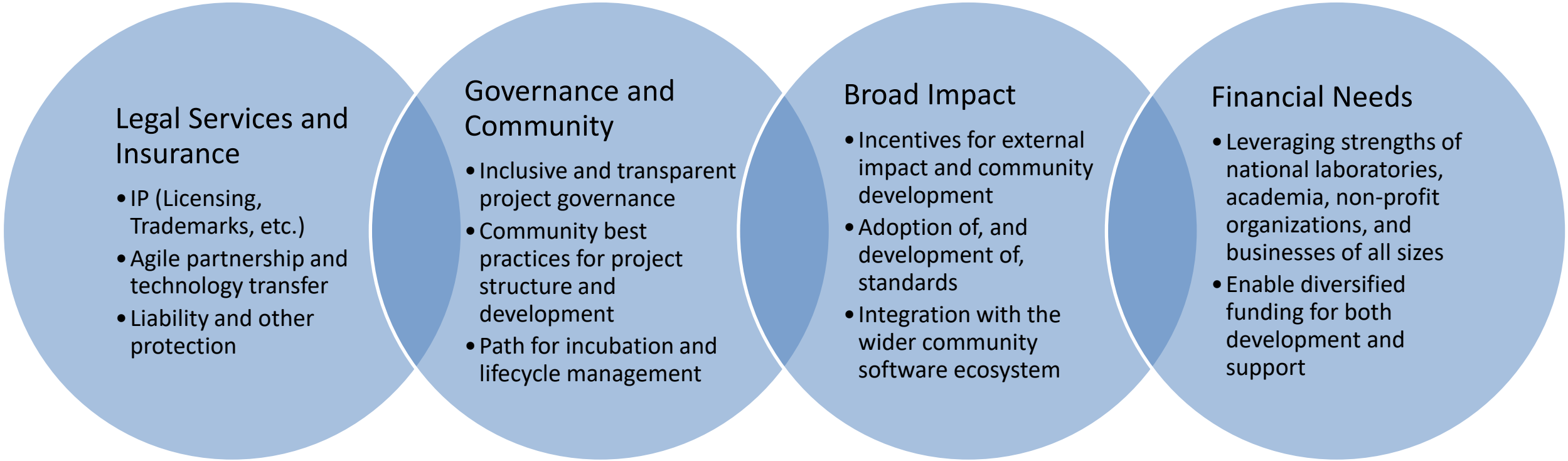
Common themes included various technical capabilities and increased alignment with community best practices:

- Data management
- Modern development tools
- Workflows and integration
- Community-aligned processes
- Machine learning
- Sparsity support
- Accelerator optimization

This slide summarizes themes noted in the RFI responses and is ***not*** comprehensive. No endorsement, recommendation, or favoring is intended or implied.

ASCR Software-Stewardship RFI: Components of Sustainable Models

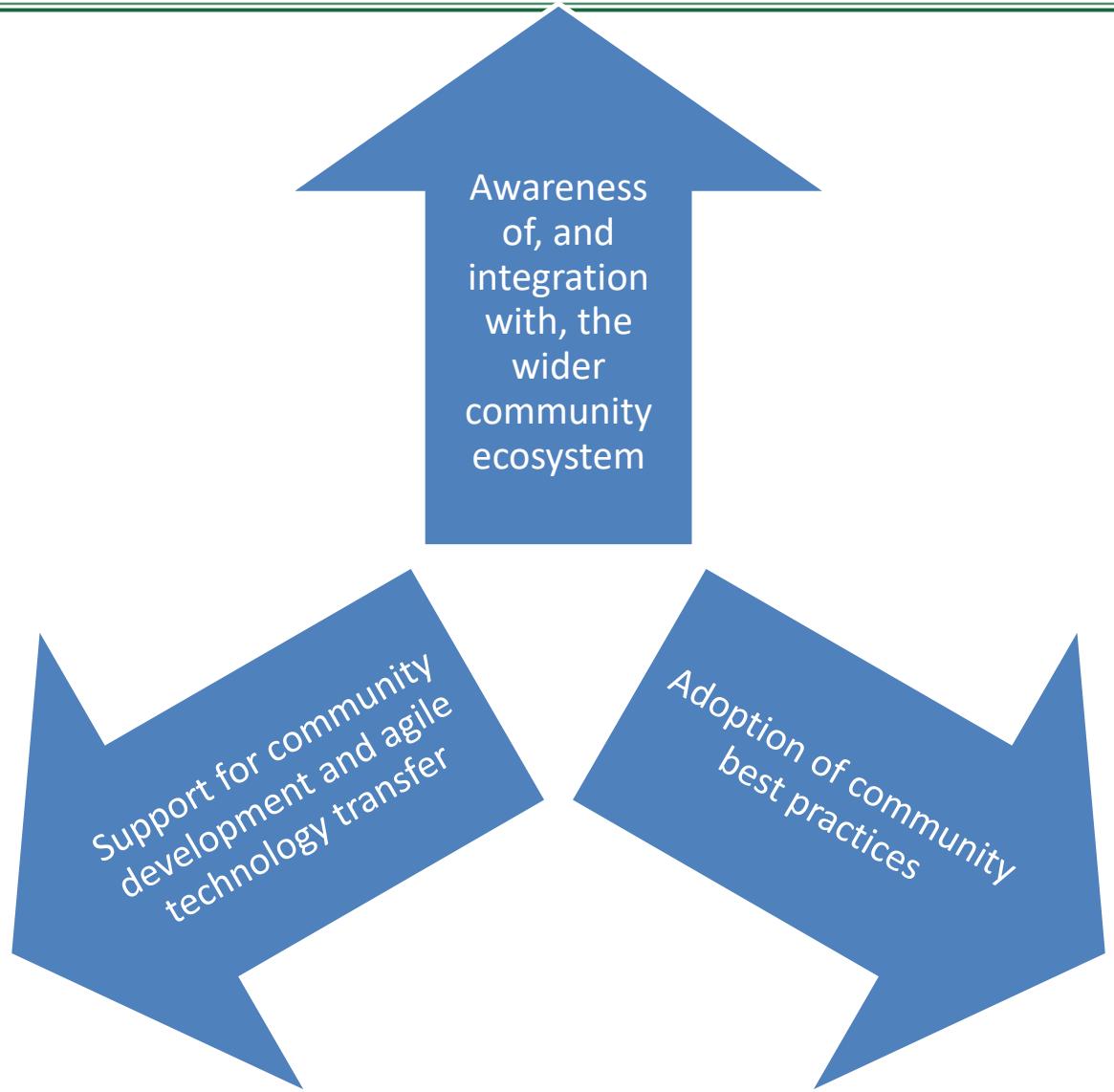
Requirements, barriers, and challenges to technology transfer, and building communities around software projects, including forming consortia and other non-profit organizations: How to encourage sustainable, resilient, and diversified funding and development models for the already-successful software within the ecosystem. What are the important characteristics and components of sustainable models for software for scientific and high-performance computing?



This slide summarizes themes noted in the RFI responses and is ***not*** comprehensive. No endorsement, recommendation, or favoring is intended or implied.

ASCR Software-Stewardship RFI: Factors Leading to Successful Models

Requirements, barriers, and challenges to technology transfer, and building communities around software projects, including forming consortia and other non-profit organizations: What development practices and other factors tend to facilitate successful establishment of these models?



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