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.

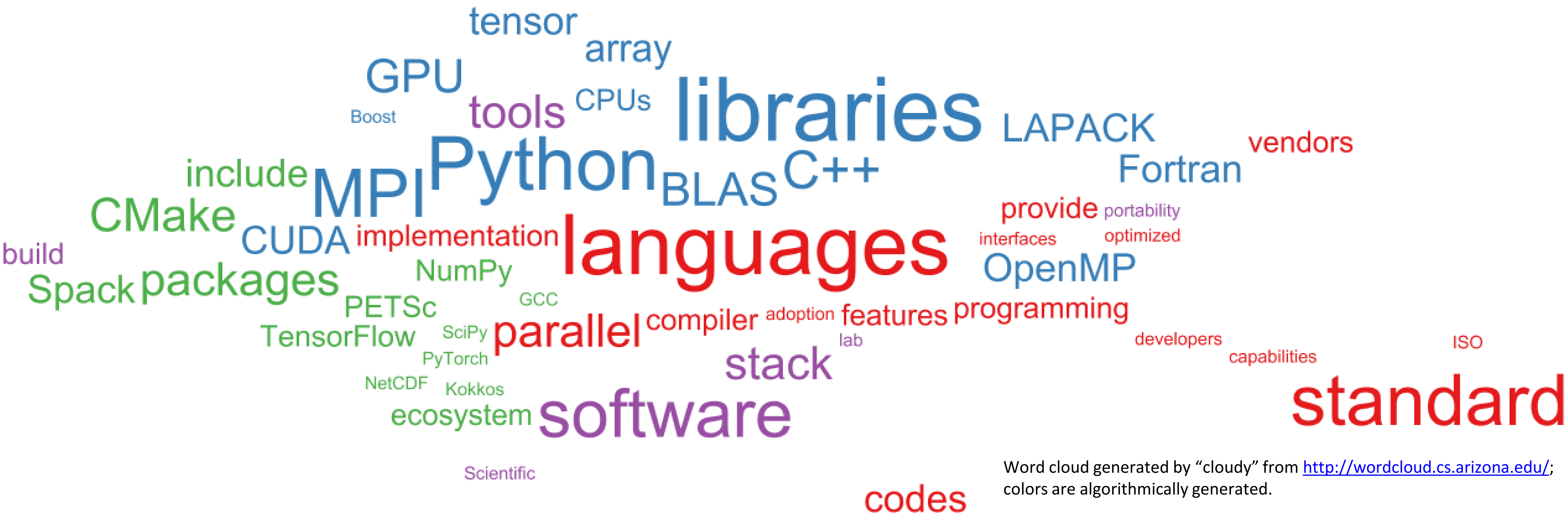
(*) Counting the two independently-authored submissions from SNL separately.

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

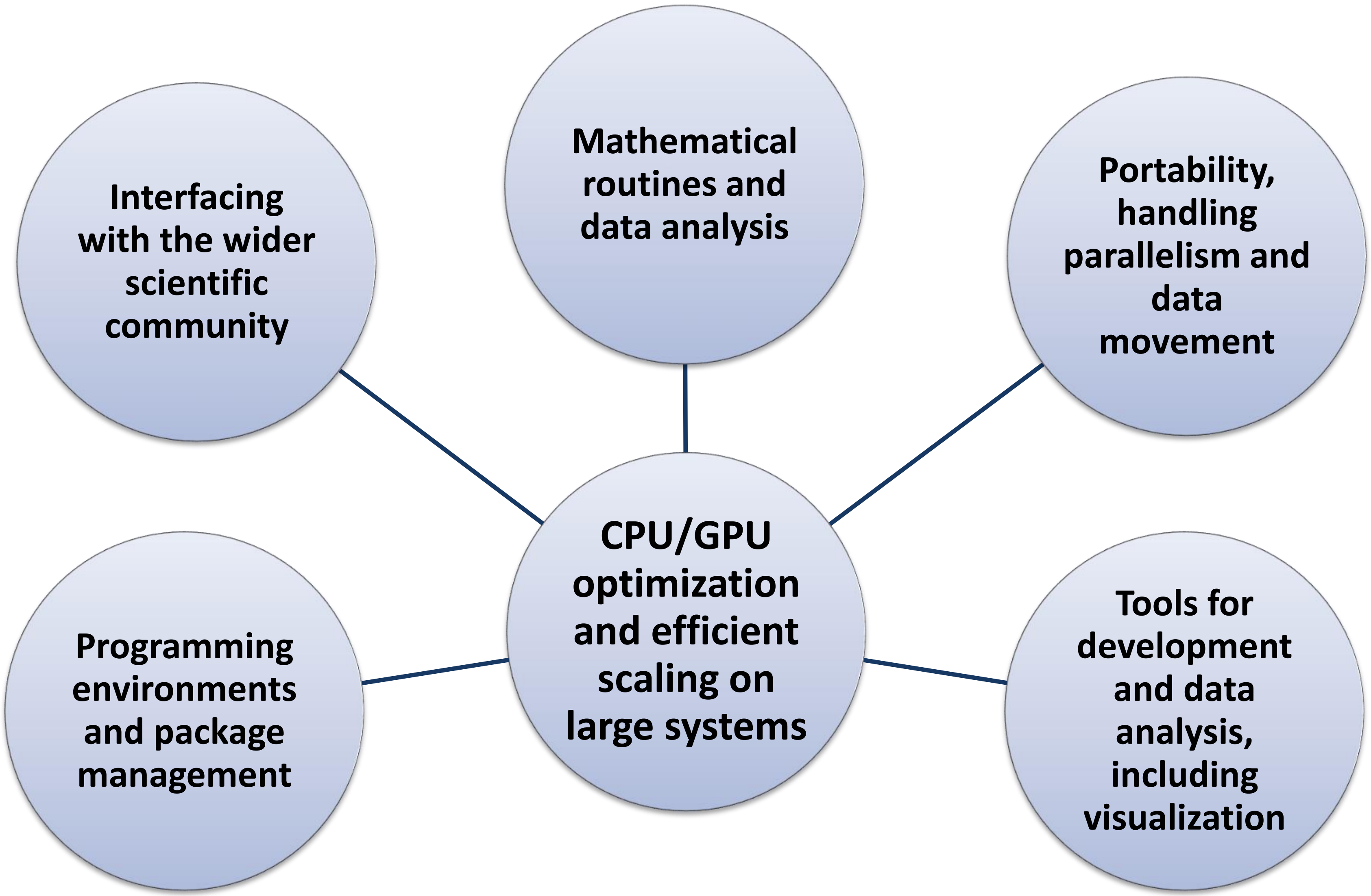
Software dependencies and requirements: What software packages and standardized languages or Application Programming Interfaces (APIs) are current or likely future dependencies for your relevant research and development activities?



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

ASCR Software-Stewardship RFI: Key Capabilities Provided by Dependencies

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



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: 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

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ASCR Software-Stewardship RFI: Dependency Risks and Mitigation Strategies

Software dependencies and requirements: What are the most-significant foreseeable risks associated with these dependencies and what are your preferred mitigation strategies?

Risks

- Library dependencies without stable support
- Support for many combinations of (upcoming, current, and past) systems and libraries, including packaging/container/build functionality

Mitigation Strategies

- Leveraging and participating in larger communities
- Defining APIs (Application Programming Interfaces)
- Package management
- Automated, regular testing
- Good documentation
- Source access

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Practices related to the security and integrity of software and data: What strategies and technology do you employ, or intend to employ in the foreseeable future, to ensure the security and integrity of your software and its associated provenance metadata?

Tools

- Version and access control
- Automated testing and analysis
- AI/ML-powered functionality

Practices

- Enforced standards and policies
- Good documentation
- Whole-team involvement

Community best practices, including SLSA (Supply chain Levels for Software Artifacts) and SBOM (Software Bill of Materials), are actively emerging.

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ASCR Software-Stewardship RFI: Infrastructure Requirements

Infrastructure requirements for software development for scientific and high-performance computing:

- What infrastructure requirements do you have in order to productively develop state-of-the-art software for scientific and high-performance computing?
- What are the key capabilities provided by this infrastructure that enables it to meet your needs?
- What key capabilities, which are not already present, do you anticipate requiring within the foreseeable future?

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ASCR Software-Stewardship RFI: Infrastructure Risks

Infrastructure requirements for software development for scientific and high-performance computing: What are the most-significant foreseeable risks associated with this infrastructure and what are your preferred mitigation strategies?

External Risks

- Lack of vendor support or low vendor responsiveness
- Hardware, driver, and operating-system defects and unavailability

Internal Risks

- Application and library defects
- Inability to adapt applications and libraries to new systems

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ASCR Software-Stewardship RFI: Additional Effort for Community Software

Developing and maintaining community software: What tasks are the largest contributors to that additional effort?

Community Requirements

- Supporting additional platforms
- Developing additional features
- Additional testing and performing tuning
- More comprehensive documentation and training material

Community Interaction

- Reviewing and integrating contributions
- Tracking, investigating, and resolving bug reports and feature requests
- Engaging with the community during design and decision processes
- Advertising, training, and event planning

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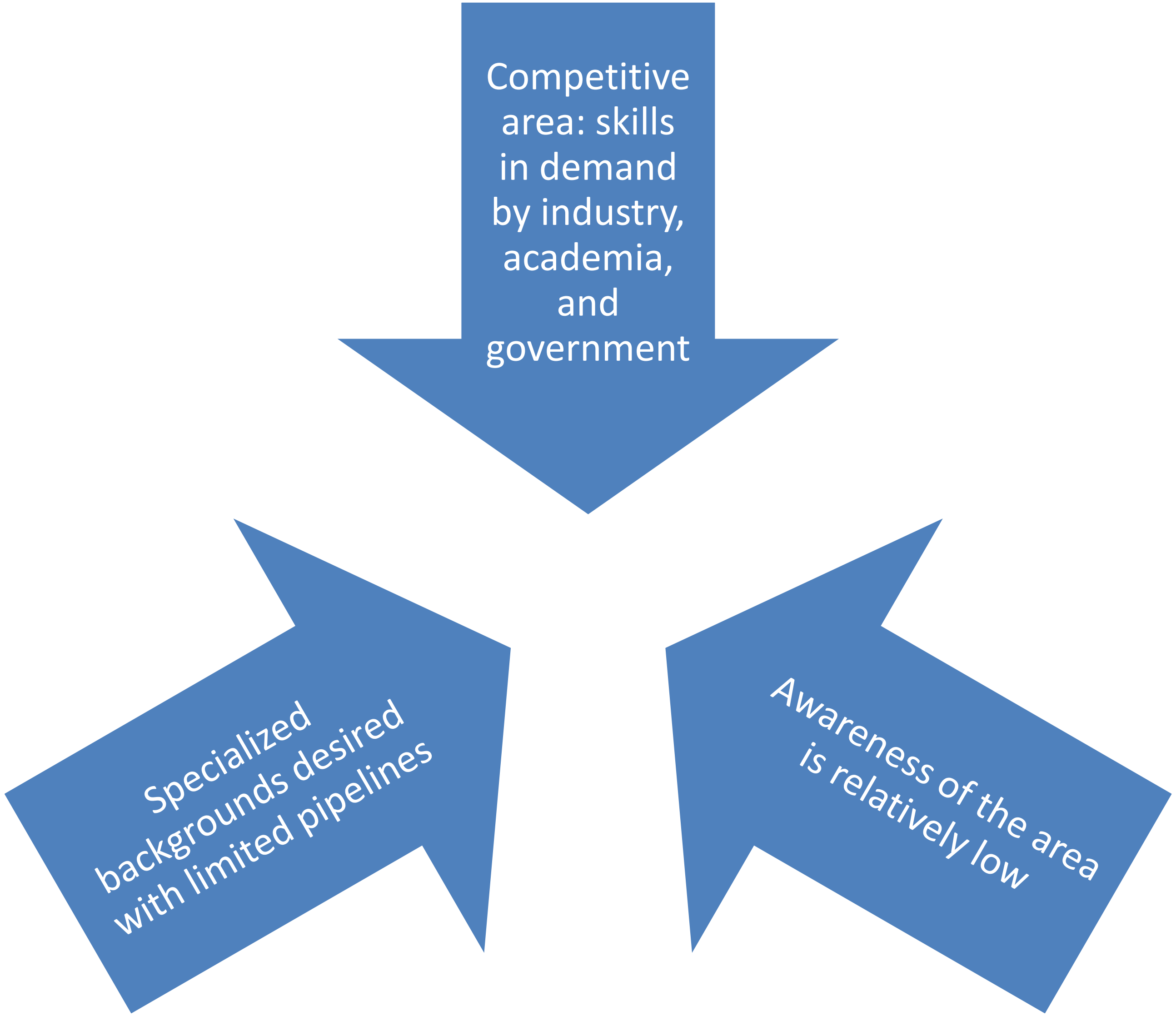
ASCR Software-Stewardship RFI: Community Software Non-Monetary Impediments

Developing and maintaining community software: What are the largest non-monetary impediments to performing this additional work?

- Maintaining additional infrastructure
- Managing additional software and process complexity
- Understanding external user requirements
- Lack of associated incentives and recognition
- Lack of time and ability to provide support commitments

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

Challenges in building a diverse workforce and maintaining an inclusive professional environment: What challenges do you face in recruiting and retaining talented professionals to develop 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: Recruitment and Retention Challenges (URG/UC)

Challenges in building a diverse workforce and maintaining an inclusive professional environment: What additional challenges exist in recruiting and retaining talented professionals from groups historically underrepresented in STEM and/or individuals from underserved communities?

Pipeline challenges

- Diversity in existing pipelines needs improvement
- Lack of awareness, training, and mentorship
- Difficulties with technology access

Recruiting practices

- Unconscious bias
- Overreliance on traditional pipelines
- Inflexible stated degree/skill requirements

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: Successful Strategies for Diversity and Inclusion

Challenges in building a diverse workforce and maintaining an inclusive professional environment:

- What successful strategies have you employed to help overcome these challenges?
- What opportunities for professional recognition and career advancement exist for those engaged in developing scientific and high-performance computing software?

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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?

Legal Services and Insurance

- IP (Licensing, Trademarks, etc.)
- Agile partnership and technology transfer
- Liability and other protection

Governance and Community

- Inclusive and transparent project governance
- Community best practices for project structure and development
- Path for incubation and lifecycle management

Broad Impact

- Incentives for external impact and community development
- Adoption of, and development of, standards
- Integration with the wider community software ecosystem

Financial Needs

- Leveraging strengths of national laboratories, academia, non-profit organizations, and businesses of all sizes
- Enable diversified funding for both development and support

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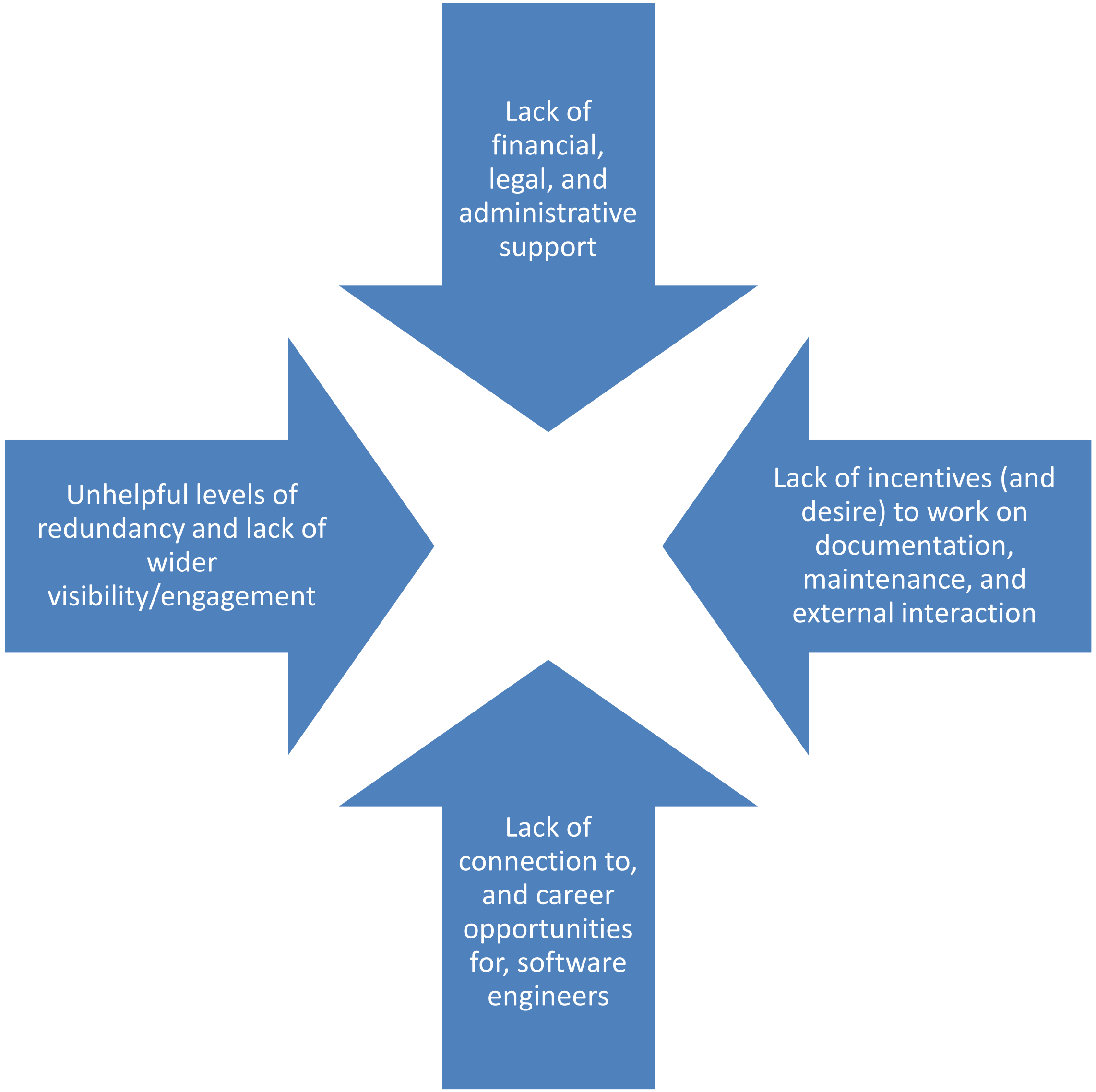
ASCR Software-Stewardship RFI: Barriers to Sustainable Models

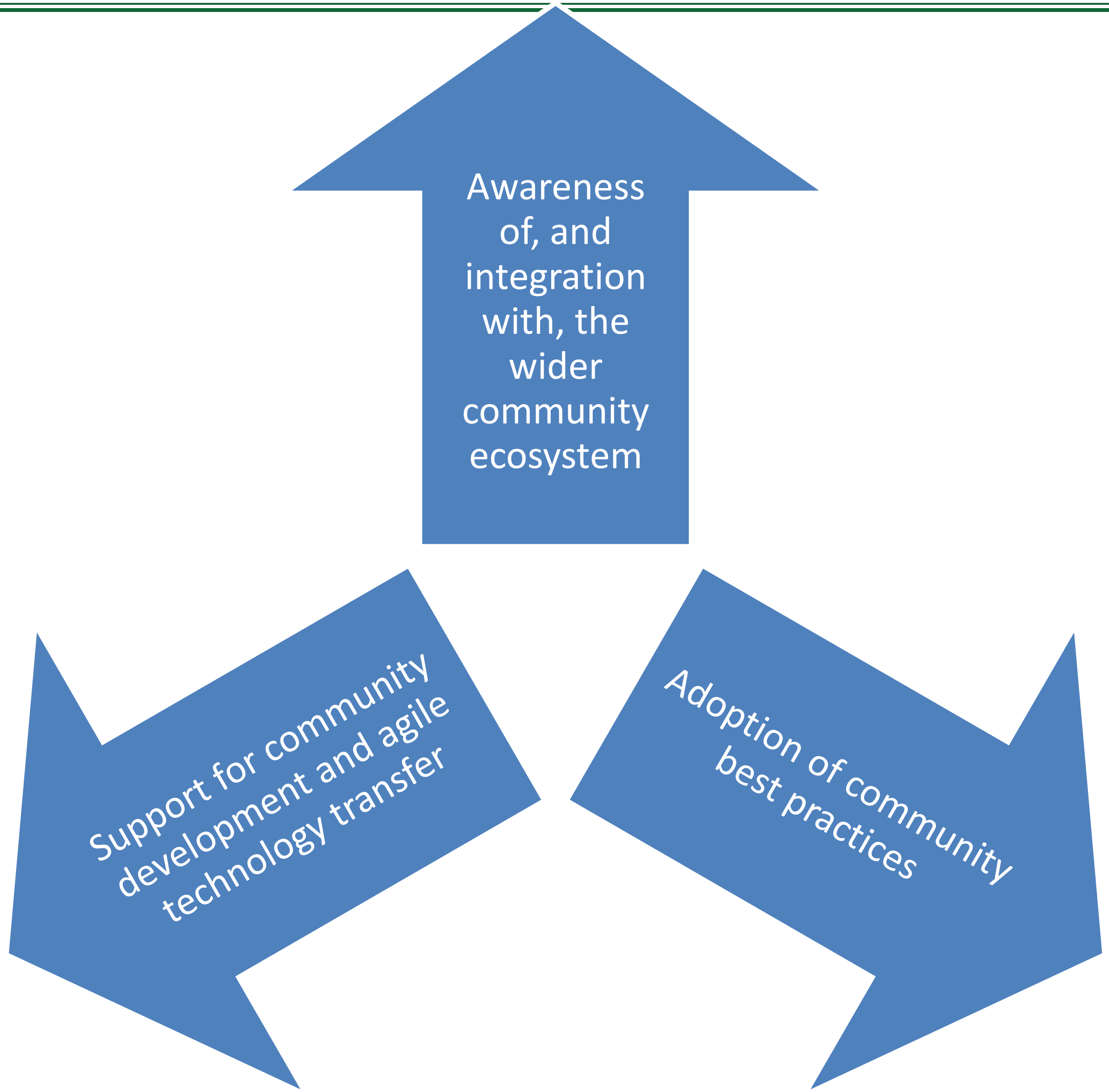
Requirements, barriers, and challenges to technology transfer, and building communities around software projects, including forming consortia and other non-profit organizations: What are key obstacles, impediments, or bottlenecks to the establishment and success of these models?



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?



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: Additional Scope

Overall scope of the stewardship effort: Are there activities that should be added to, or removed from, this list?

- ✓ 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 (including the incorporation of new capabilities)

- \+ Application engagement and support
- \+ Training on best practices for community development/management
- \+ Community outreach and networking
- \+ Legal and administrative support

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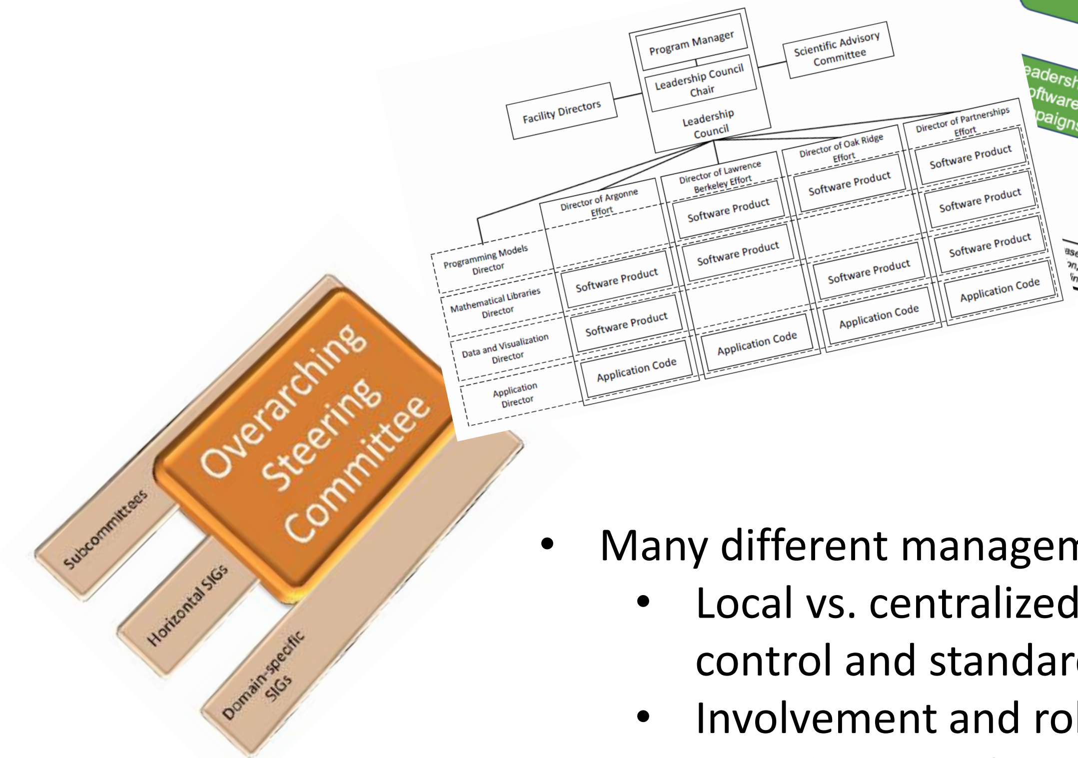
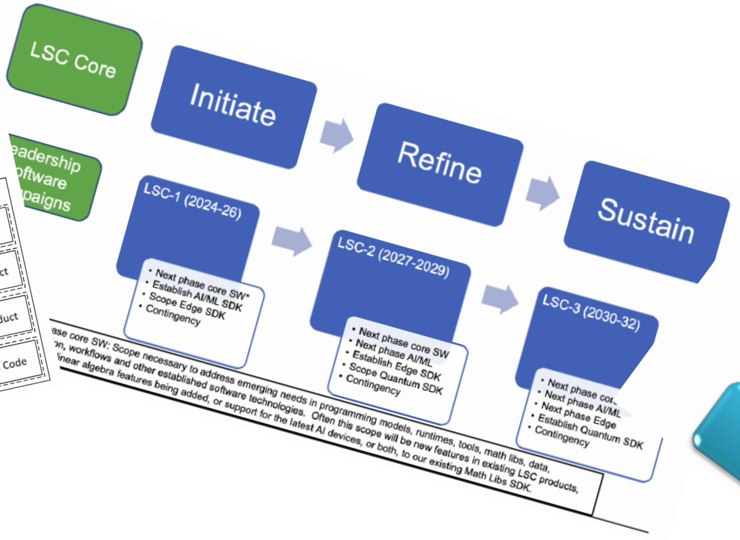
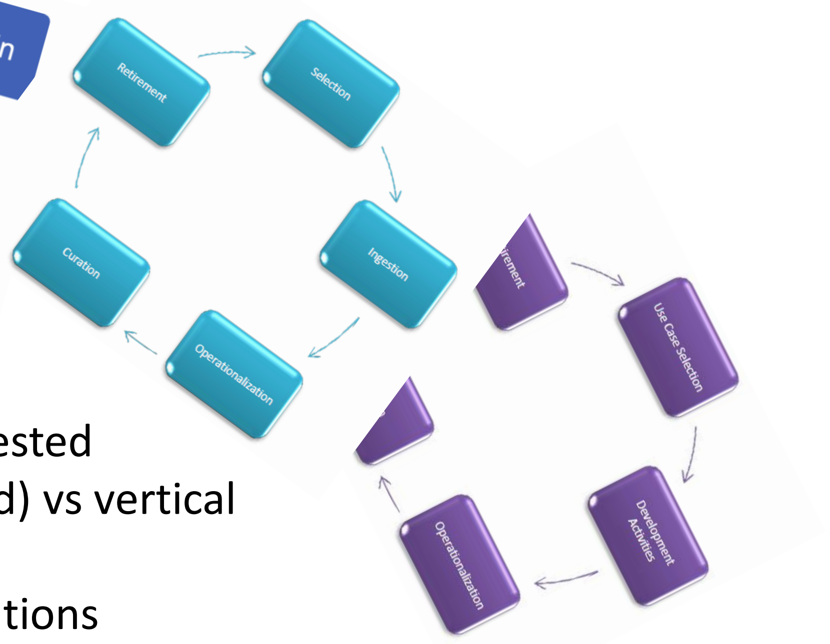
ASCR Software-Stewardship RFI: Management and Oversight

Management and oversight structure of the stewardship effort: What do you anticipate will be effective models for management and oversight of the scientific and high-performance-computing software ecosystem, and how would that management structure most-effectively interact with DOE and other stakeholders?







- Many different management structures have been suggested
  - Local vs. centralized and horizontal (domain focused) vs vertical control and standards setting
  - Involvement and roles of different kinds of organizations
  - Varied approaches to lifecycle management and curation

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: Coordination with DOE Facilities and Other Infrastructure

Management and oversight structure of the stewardship effort: How can the management structure coordinate with DOE user facilities and others to provide access to relevant testbed systems and other necessary infrastructure?

Communicate closely with DOE facilities and help enable vendor partnerships

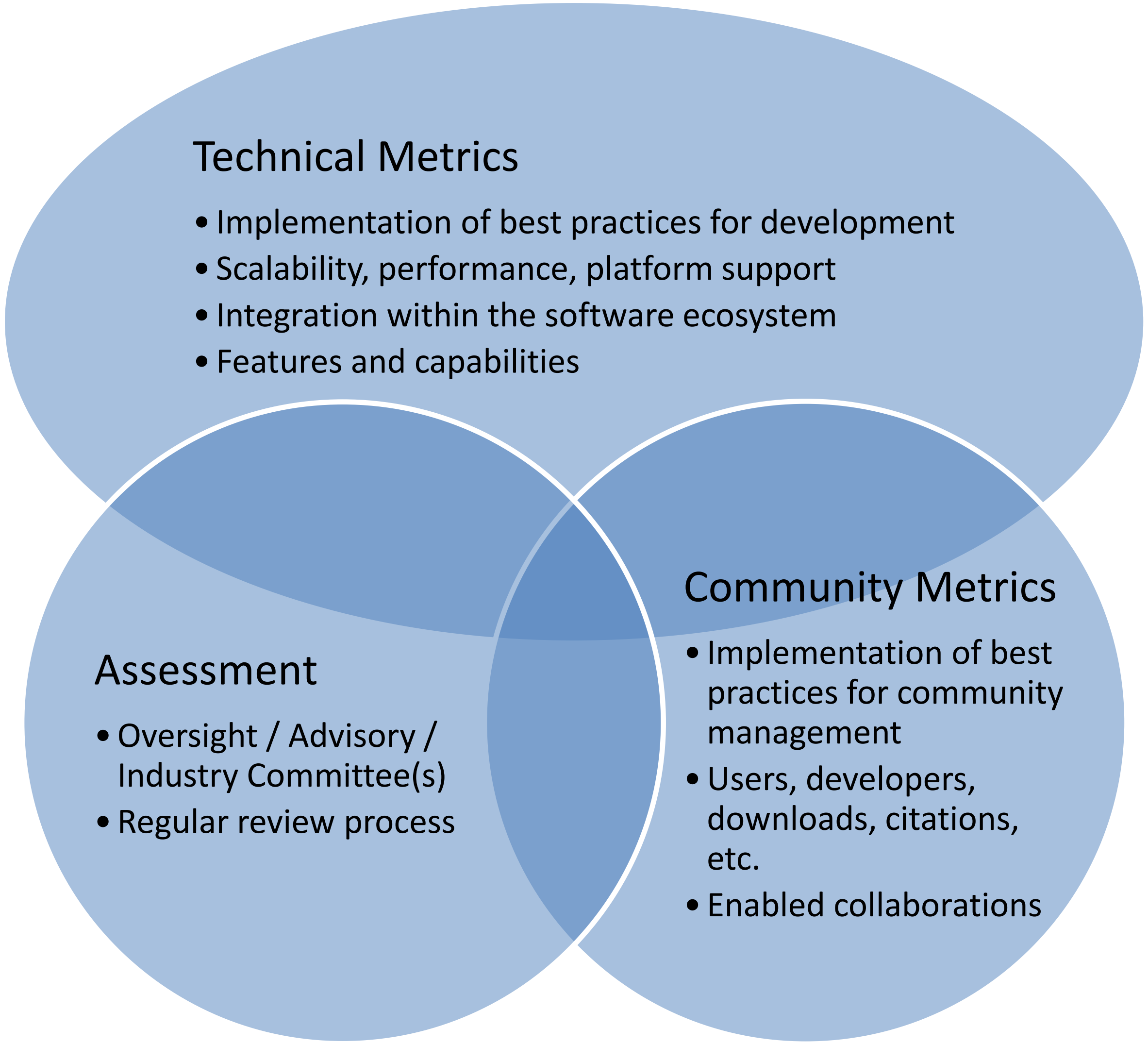
Coordinate allocation and access to both DOE and cloud/community resources

Negotiate support for automatable testing and other infrastructure services

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: Success Criteria and Assessment

Assessment and criteria for success for the stewardship effort: What kinds of metrics or criteria would be useful in measuring the success of software stewardship efforts in scientific and high-performance computing and its impact on your scientific fields or industries?



U.S. DEPARTMENT OF ENERGY | Office of Science

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ASCR Software-Stewardship: Next Steps

Next steps for ASCR regarding software stewardship:

1. Finalize the targeted scope of potential software-stewardship activities for FY23.

2. Define the relationship between those software-stewardship activities and synergistic activities in the Facilities, Research, and Advanced Computing Technologies (ACT) Divisions.

3. Pursue the definition and release of a funding opportunity, or funding opportunities, covering the targeted scope.

4. Work with ECP, ASCR facilities, and other stakeholders to enable a common understanding of how all stakeholders will contribute to the overall process.

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

Home Agenda Video Presentations Accepted Position Papers Position Paper Submission Contacts

ASCR Workshop on Reimagining Codesign

Sponsored by the U.S. Department of Energy,
Office of Advanced Scientific Computing Research

March 16-18, 2021
11:00 am to 5:00 pm ET

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

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ASCR Workshop on Reima[...]ing Codesign

Sponsored by the U.S. Department of E[...] Office of Advanced Scientific Comp

March 16-18, 2021

The Video Presentations page has videos of most plenary sessions.

Day 1

Introduction and Workshop Logistics

Hal Finkel - Welcome and Opening Remarks

Barbara Helland - View from Department of Energy

Keynote Speaker – Neil Thompson, MIT

Catherine Schuman - Top-Down Neuromorphic Hardware Co- Design via Machine Learning and Simulation

Ryan Grant - Co-design of System Software for Compute Accelerators and SmartNICs

Thomas Flynn - Real-time data-driven codesign of hardware and software for analysis of high-throughput scier

Eric Cheng - Project 38: Innovative Architectures for High-Performance Computing Systems

Andreas Gerstlauer - Algorithm-Architecture Codesign for Irregular and Sparse Problems

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

Home Agenda Video Presentations **Accepted Position Papers** Position Paper Submission Contacts

ASCR Workshop on Reimagining Codesign

Sponsored by the U.S. Department of Energ… …e of Advanced Scientific Computing

March 16-18, 2021

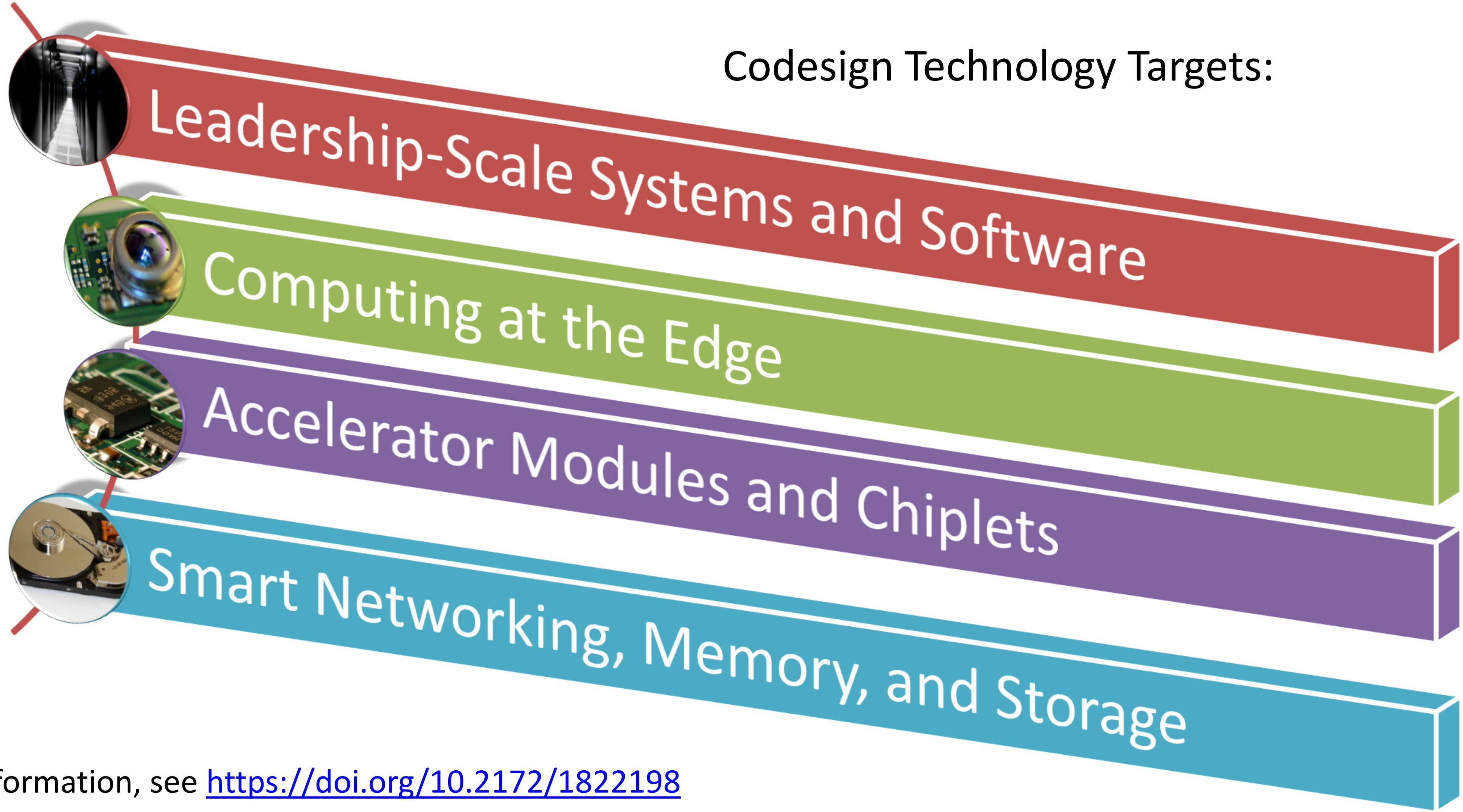
The Accepted Position Papers page has the 86 accepted position papers.

Author	Institutional Affiliation	
Alex Aiken	Stanford/SLAC	…odesign
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:

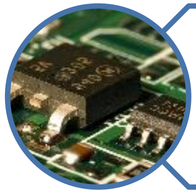


For more information, see https://doi.org/10.2172/1822198

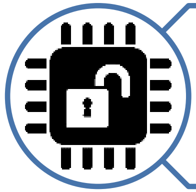
ASCR Workshop on Reimagining Codesign: Enabling Technology Factors

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

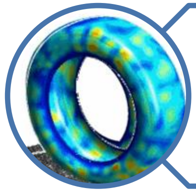
Enabling Key Technology Factors:



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

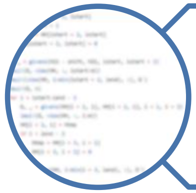


Open-source hardware designs allowing open, low-risk collaboration among academics, laboratories, and industry



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

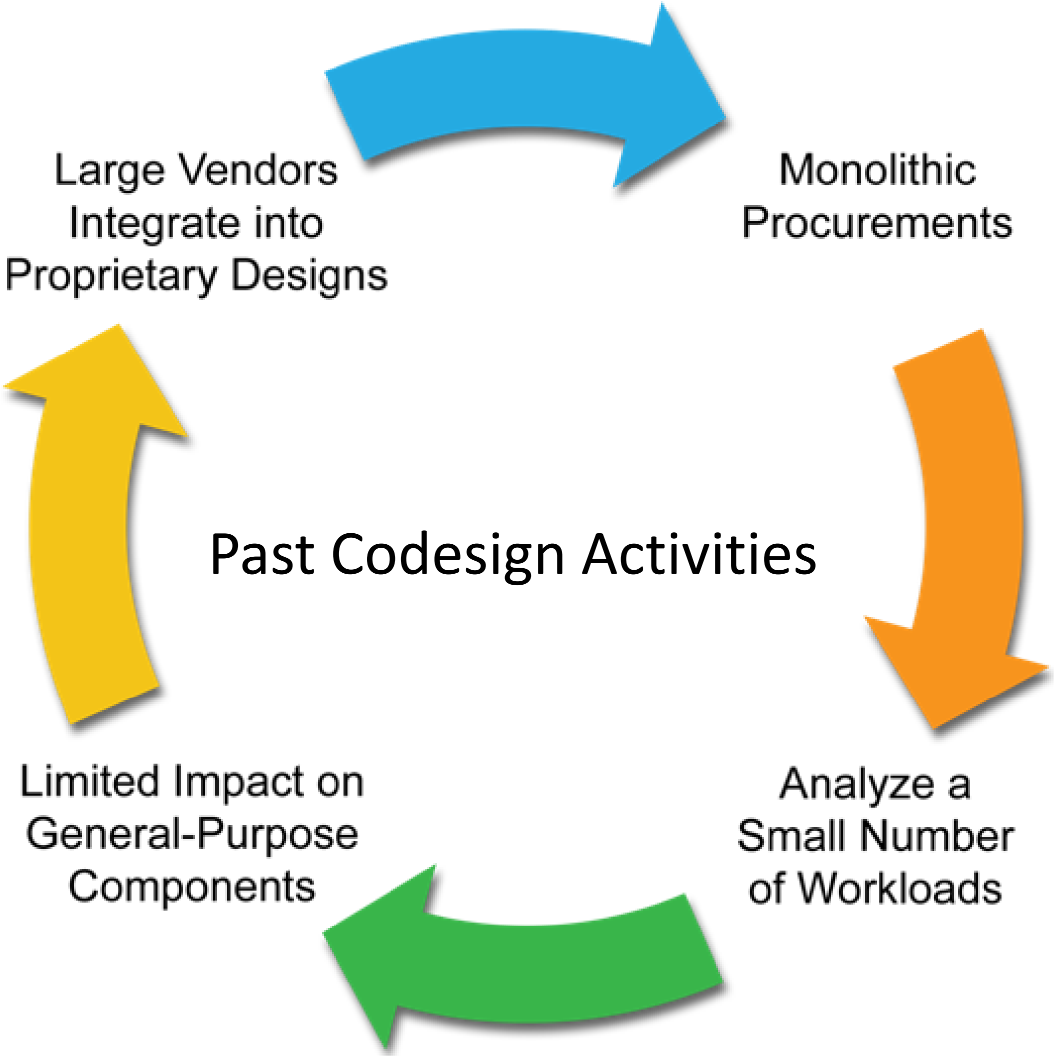


The foundations laid in pursuit of exascale computing have generated applications capable of using first-generation heterogeneous GPU computing resources through **portable programming models and adaptive system software**

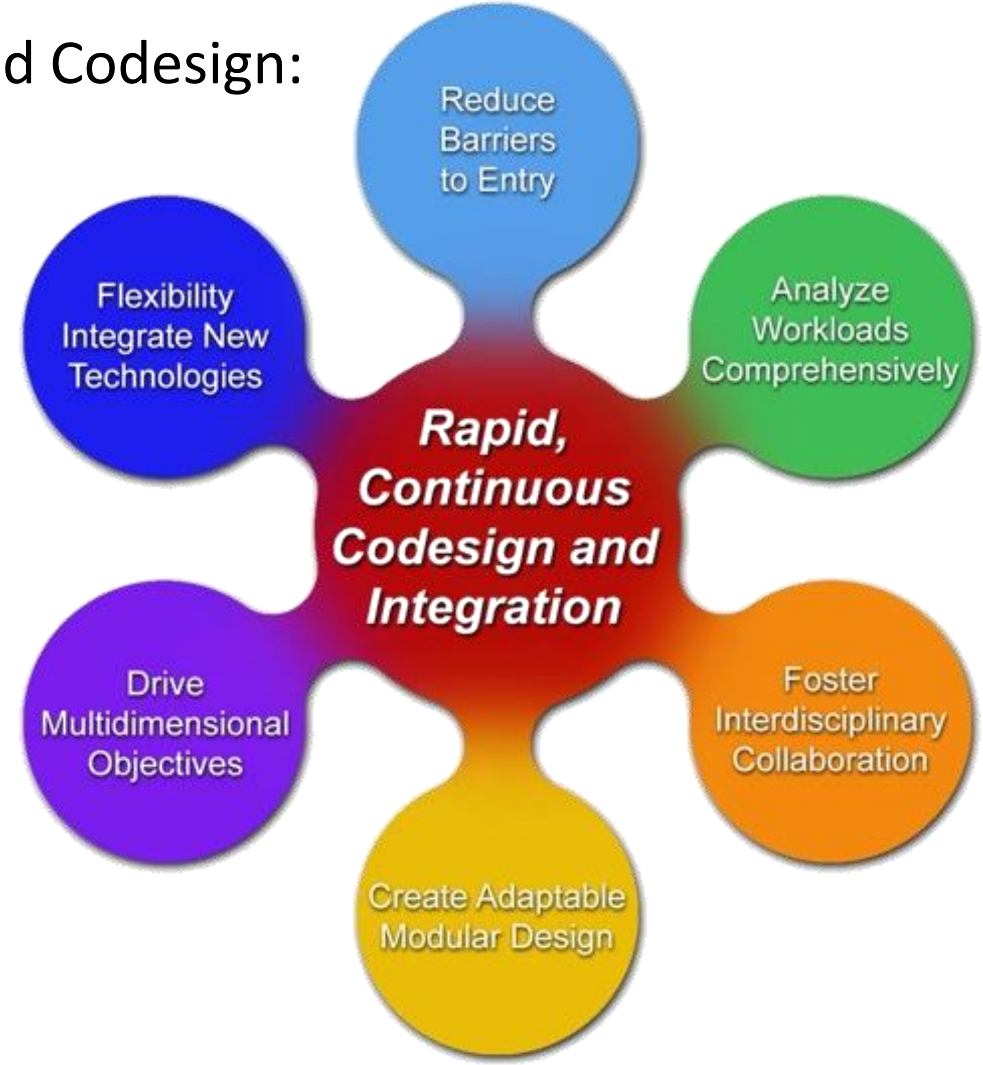
For more information, see https://doi.org/10.2172/1822198

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

ASCR Workshop on Reimagining Codesign: PRDs

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

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

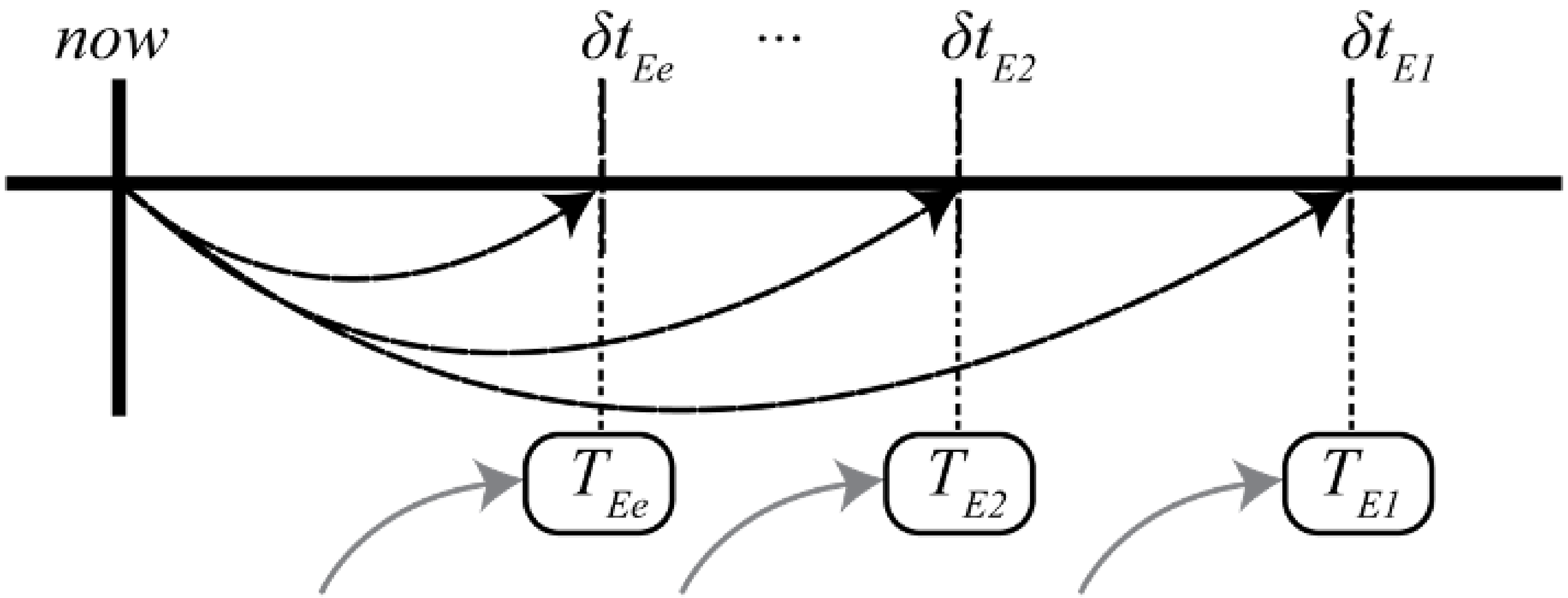
Key Questions: What are the quantitative tools that are practical, accurate, and applicable to codesigning various layers of the hardware/software stack and of data-driven, dynamic, irregular workflows, such as those occurring in experimental science or AI/machine learning workloads?

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 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.

Parallel Discrete Event Execution on High Performance Computing Platforms

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.

Discrete event execution style is vastly different from most traditional supercomputing-based simulations

Translates to

- Different optimizations
- Different communication patterns
- Different latency needs
- Different bandwidth needs
- Different buffering requirements
- Different scheduling needs
- Different synchronization requirements
- Different flow control schemes

PDES needs a different runtime

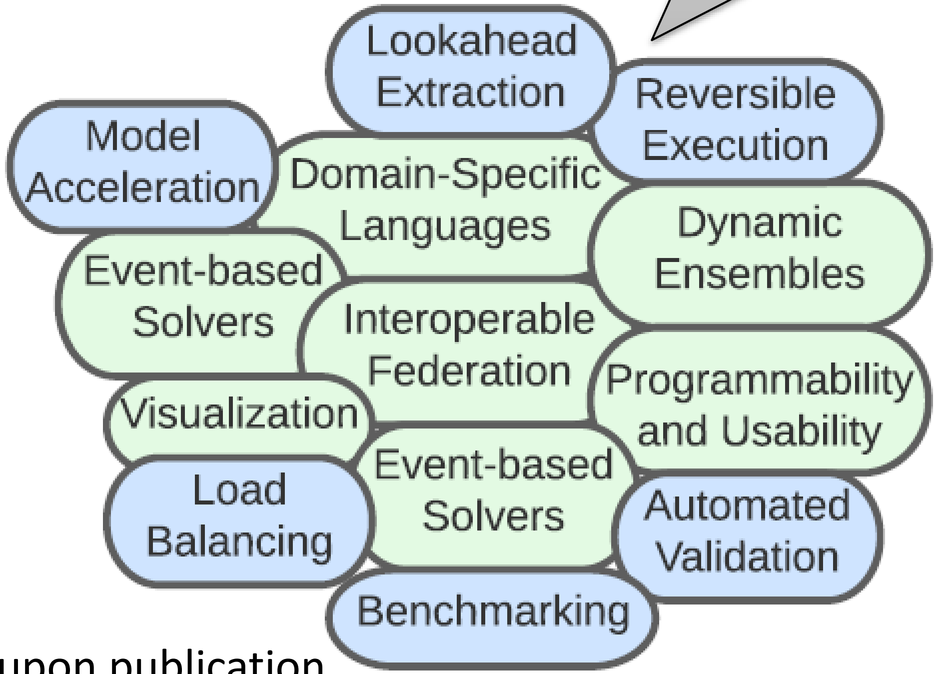
- Qualitatively different runtime infrastructure, optimized and tuned for discrete event applications

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/10.2172/1855274 upon publication.