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

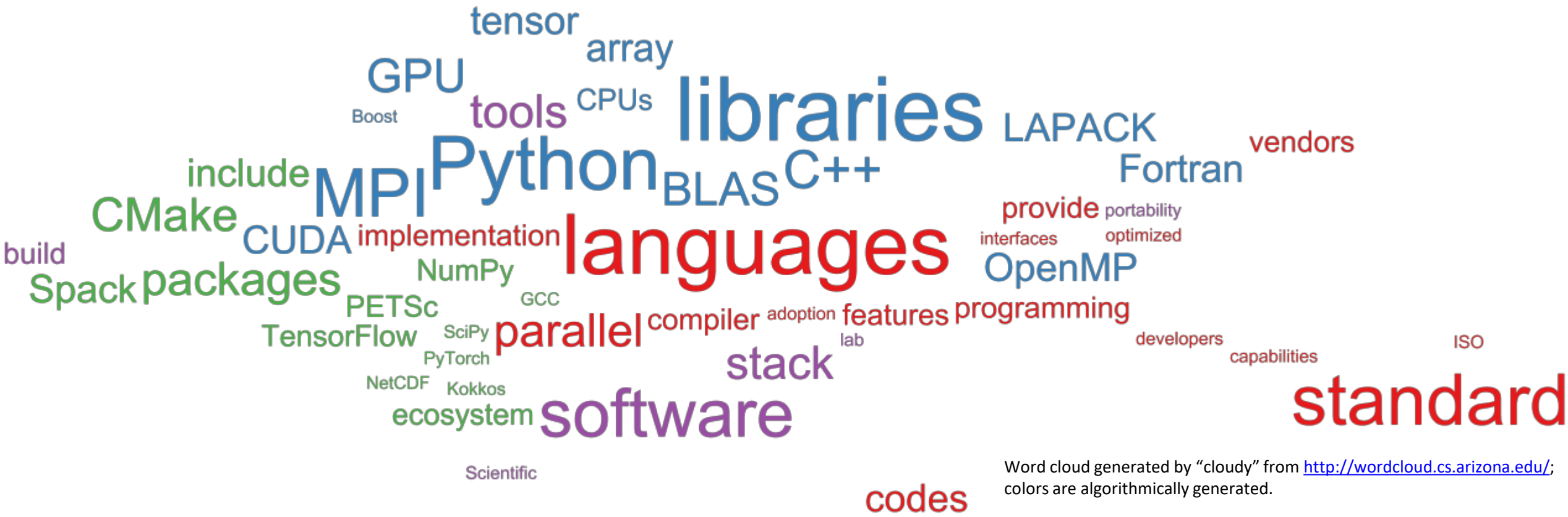
Note: The following slides summarize themes noted in the RFI responses, and they are ***not*** comprehensive. Their purpose is to inspire interest in reading the RFI responses, available at https://doi.org/10.2172/1843576. No endorsement, recommendation, or favoring is intended or implied.

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

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.

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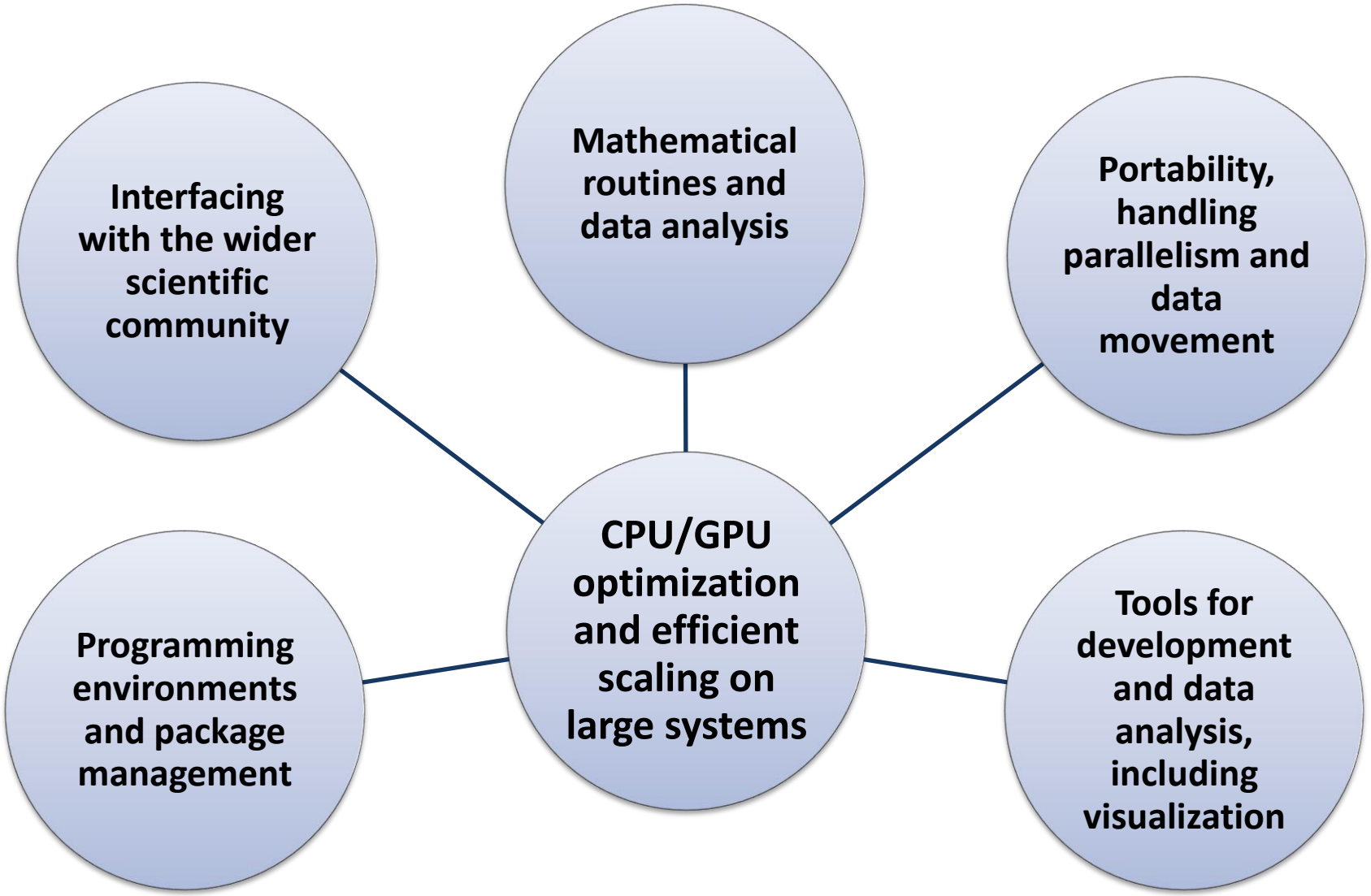
ASCR Software-Stewardship RFI: Key Capabilities Provided by Dependencies

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

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ASCR Software-Stewardship RFI: Dependency Risks and Mitigation Strategies

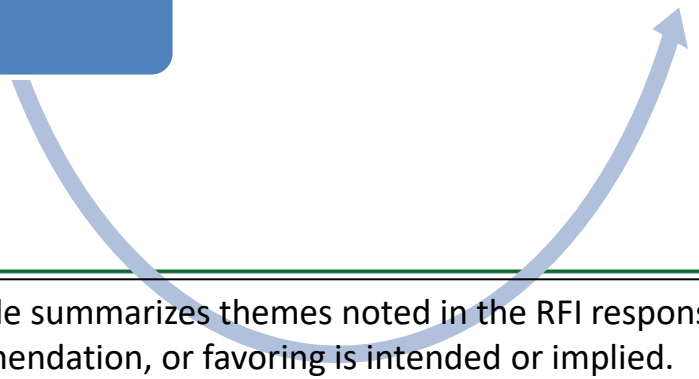
Software dependencies and requirements: What are the most-significant foreseeable risks associated with these dependencies and what are your preferred mitigation strategies?

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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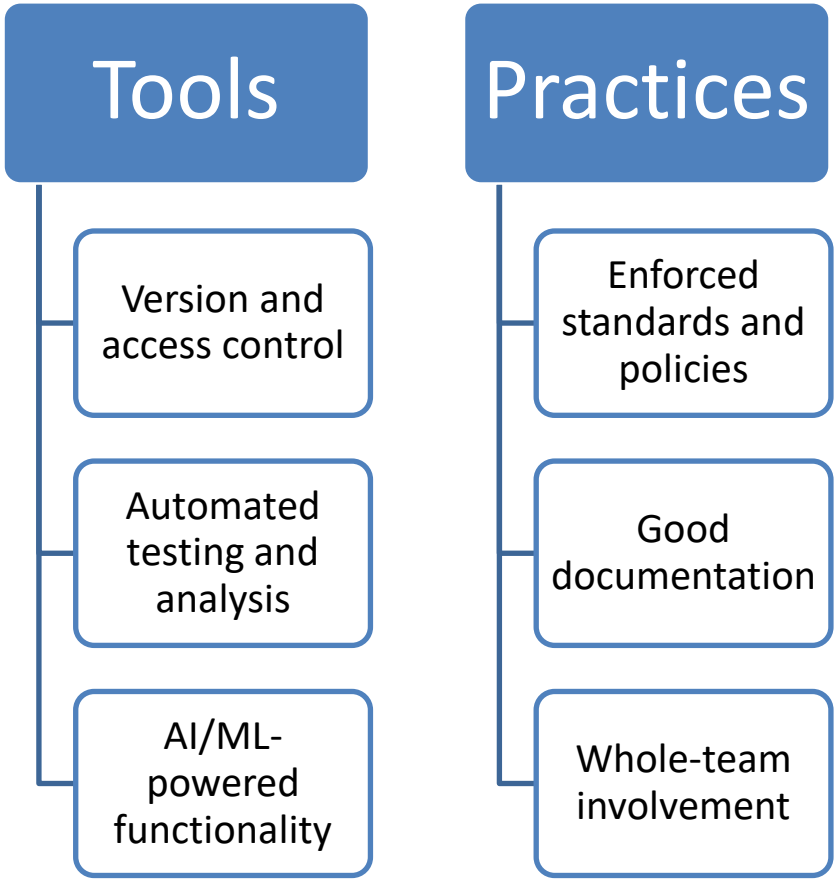
ASCR Software-Stewardship RFI: Strategies and Technologies for Software Integrity

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?



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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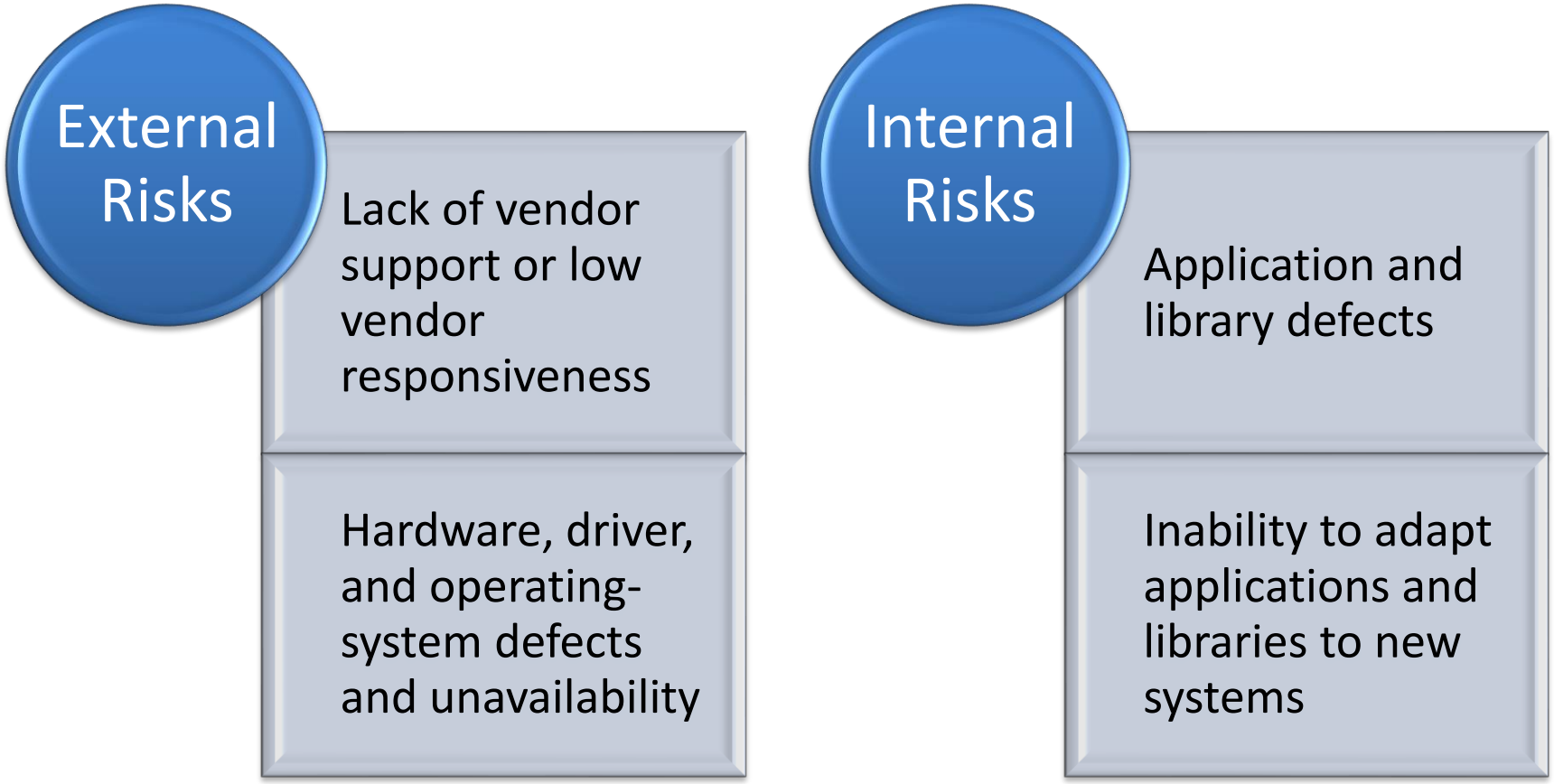
ASCR Software-Stewardship RFI: Infrastructure Risks

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?



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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

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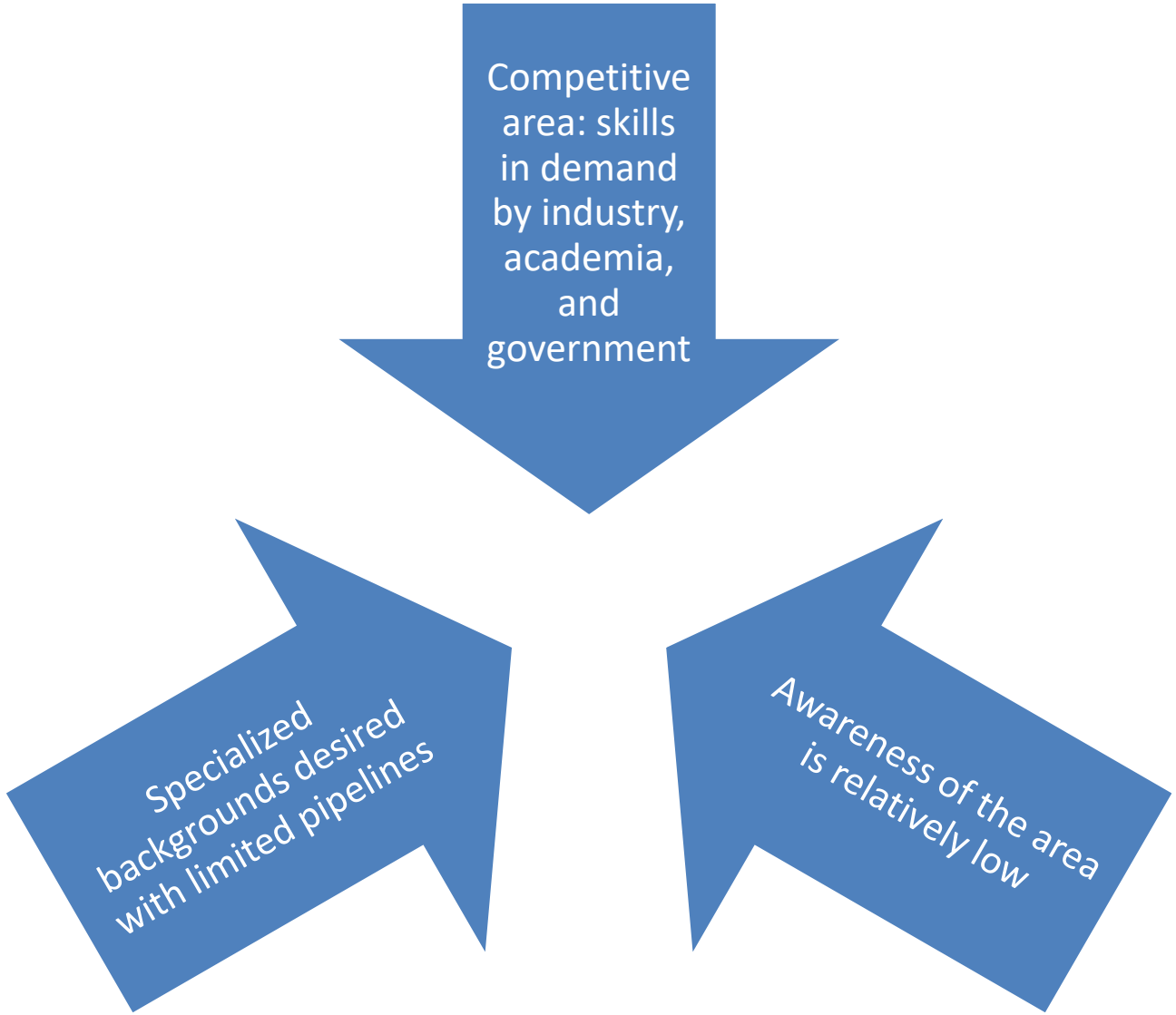
ASCR Software-Stewardship RFI: Recruiting and Retention Challenges

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?



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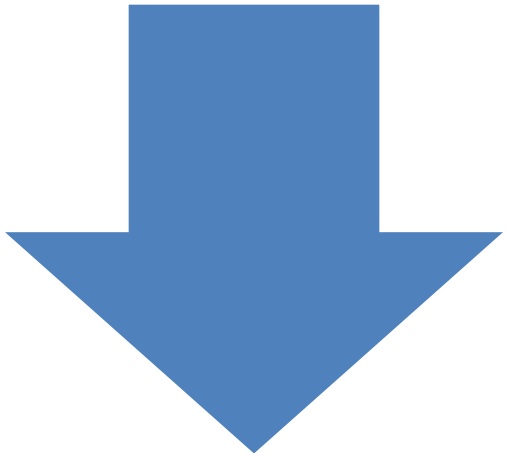
ASCR Software-Stewardship RFI: Recruitment and Retention Challenges (URG/UC)

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?

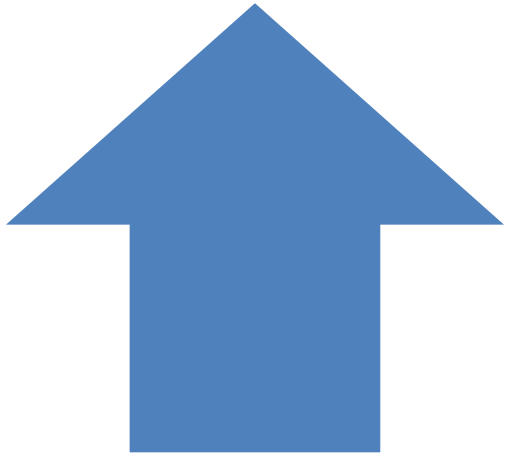


Pipeline challenges

- 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



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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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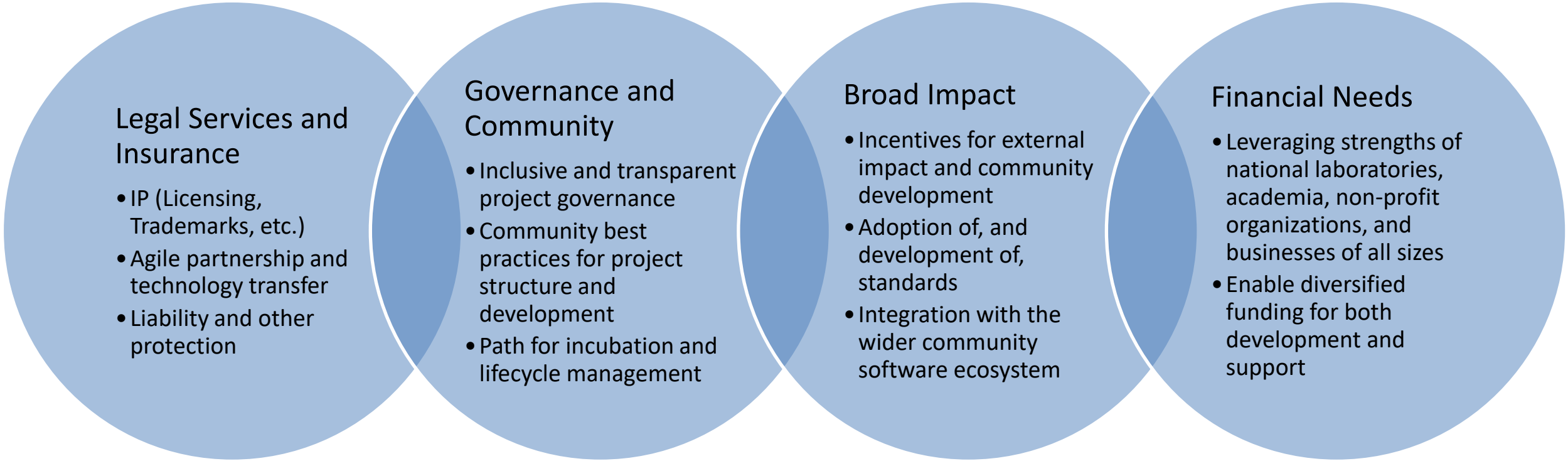
ASCR Software-Stewardship RFI: Components of Sustainable Models

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?



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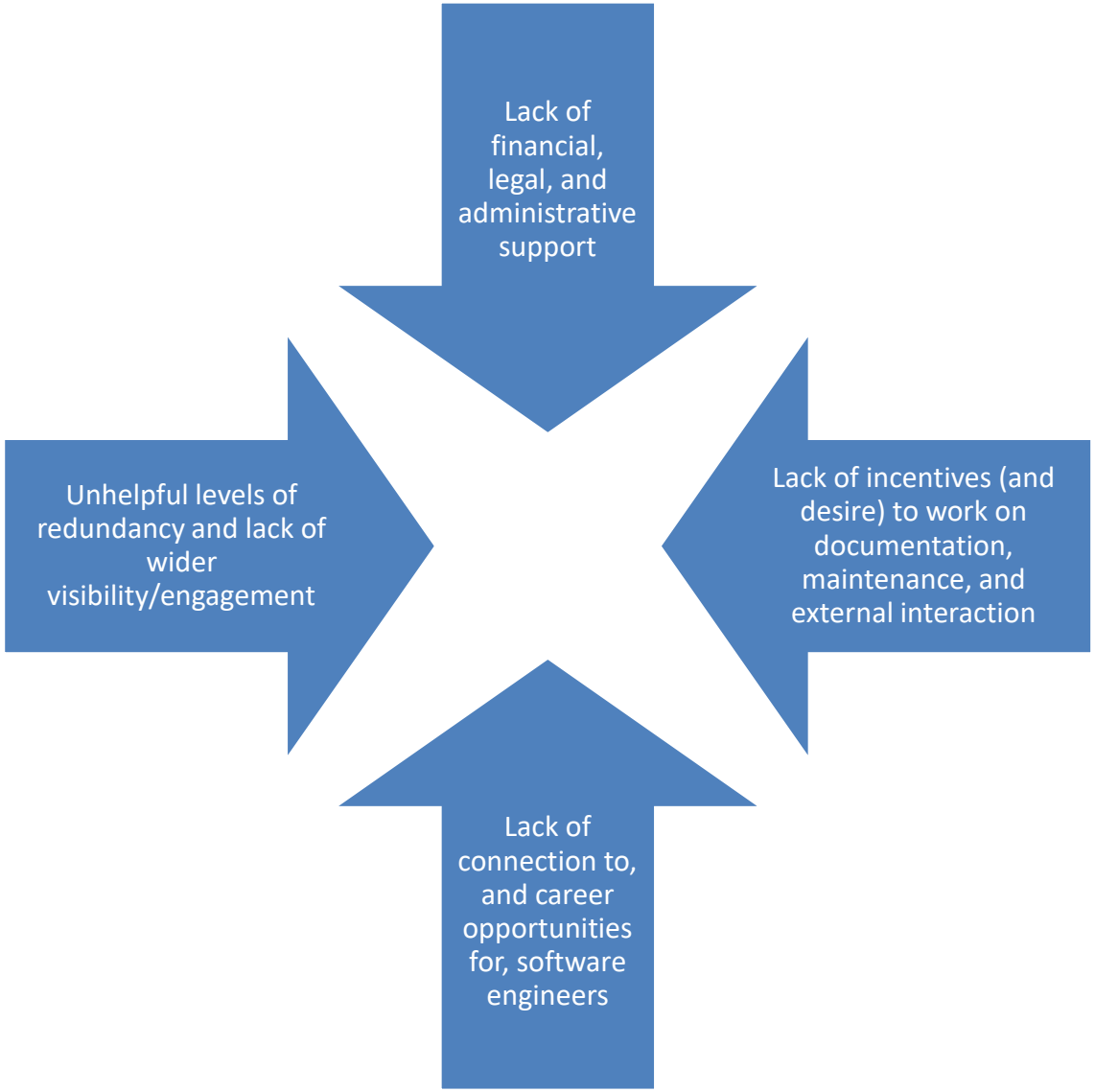
ASCR Software-Stewardship RFI: Barriers to Sustainable Models

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?



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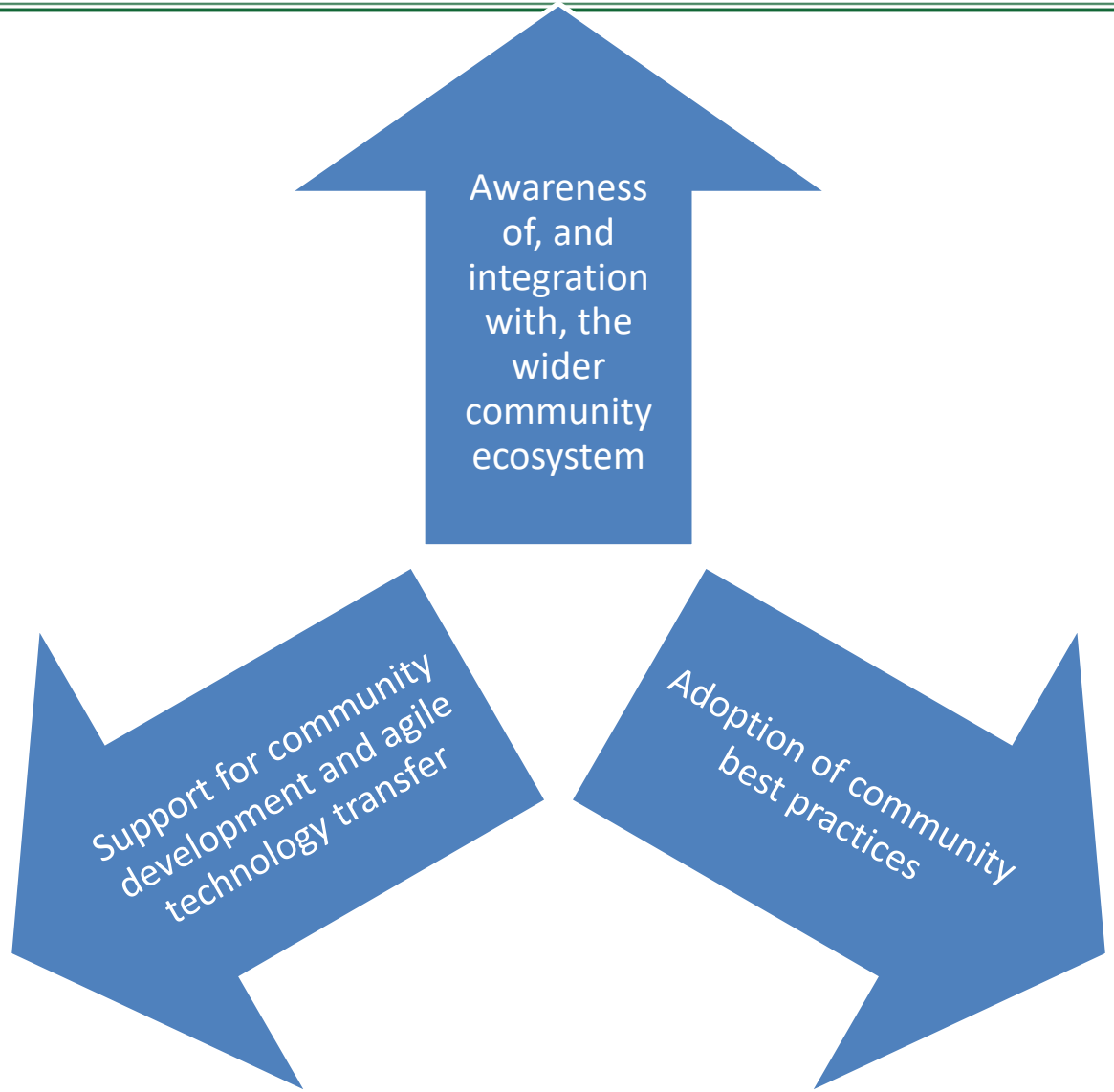
ASCR Software-Stewardship RFI: Factors Leading to Successful Models

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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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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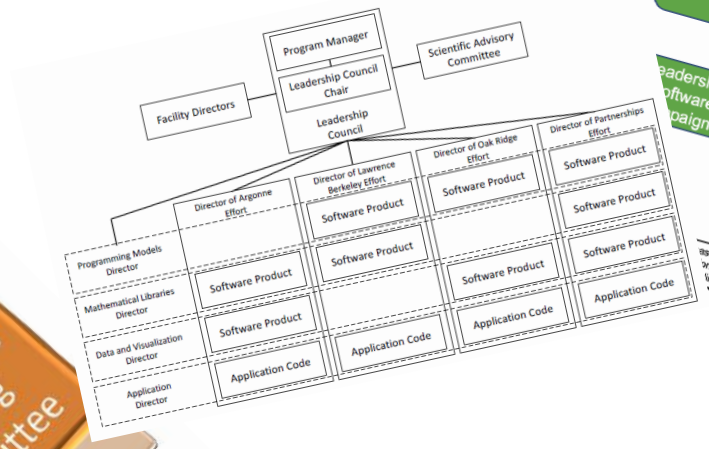
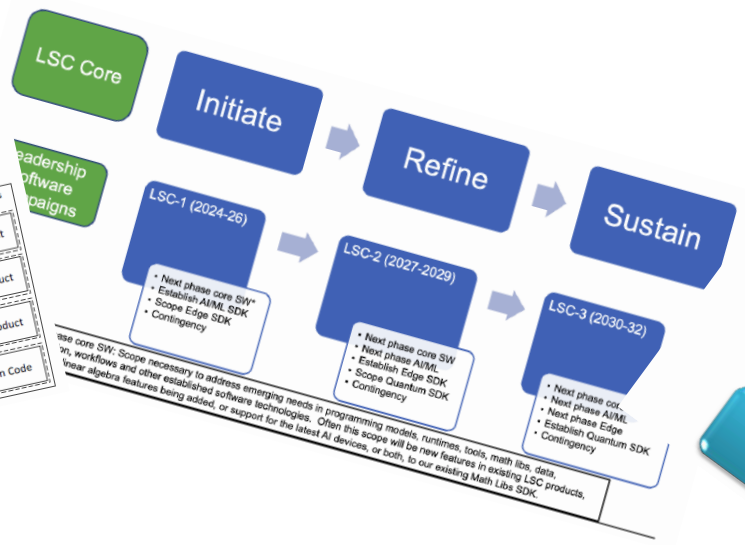
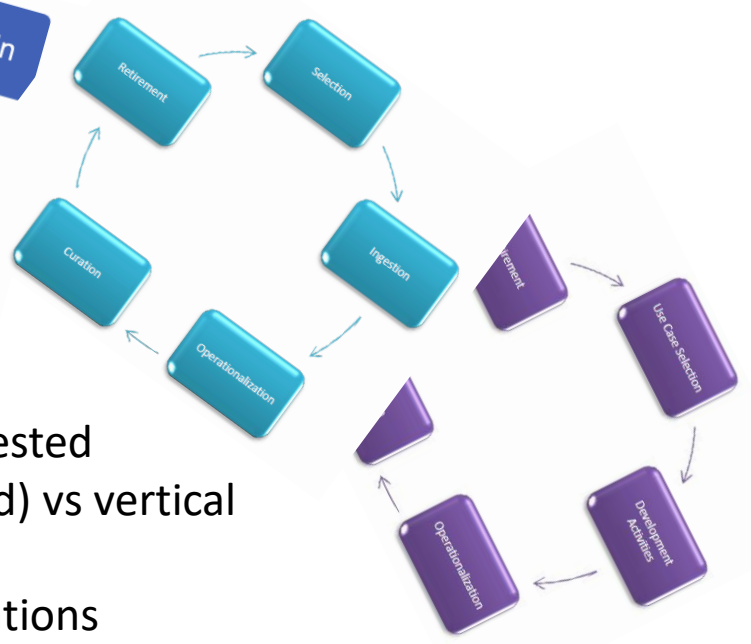
ASCR Software-Stewardship RFI: Management and Oversight

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

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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

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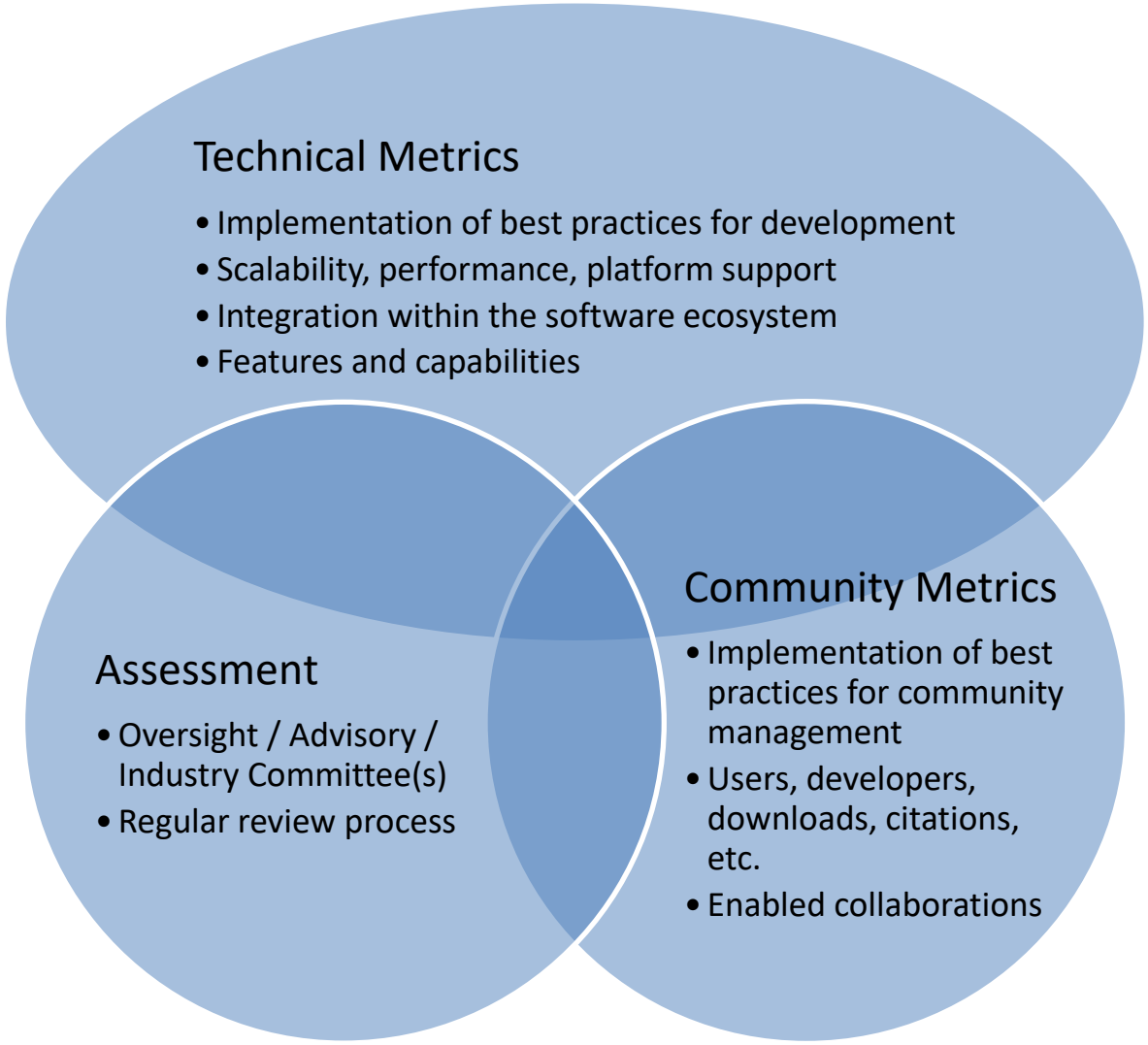
ASCR Software-Stewardship RFI: Success Criteria and Assessment

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?



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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.