Transition Report

January 13, 2020

Roscoe Giles

Outline

- Charge
- Subcommittee Activities
- Findings and Recommendations
- Discussion

Charge: Subcommittee Charge Elements

- **Examine**:
  - ECP lessons learned for **managing large collaborations**,
  - ASCR's historic **fundamental research investments** in applied mathematics, computer science and computational partnerships at the National Labs,
  - **new Research and Development priorities** in artificial intelligence, quantum information systems and strategic computing.
- **Recommendations (R):**
  - for **capturing the lessons learned** from ECP
  - **supporting** the software and hardware technologies and application development from ECP activities
  - informing ASCR's **future investment strategy** for its basic research programs

Subcommittee Members

Jay Bardhan, GlaxoSmithKline 	Richard Lethin, Reservoir Labs (ASCAC) 
Alan Edelman, MIT 	David Levermore, UMD, (ASCAC) 
Roscoe Giles, Boston U. (chair) 	Juan C. Meza, NSF (UC Merced) 
Fred Johnson, DOE/Retired 	Dan Reed, U. Utah (ASCAC) 
Alexandra Landsberg, ONR 	

Subcommittee Activities

- Stakeholder Interviews [13]

  Math & CS Researchers in and out of DOE, ECP Leaders, Lab Staff and Leaders, SC AD's & Program officers, CSGF Alumni & Fellows

- Community Meetings [3]

  Co-Loc @ ORNL and DC AI Town Halls & SC19 BoF

- Reading Reports [∞]
- Subcommittee meetings [39…]

Overview

Context

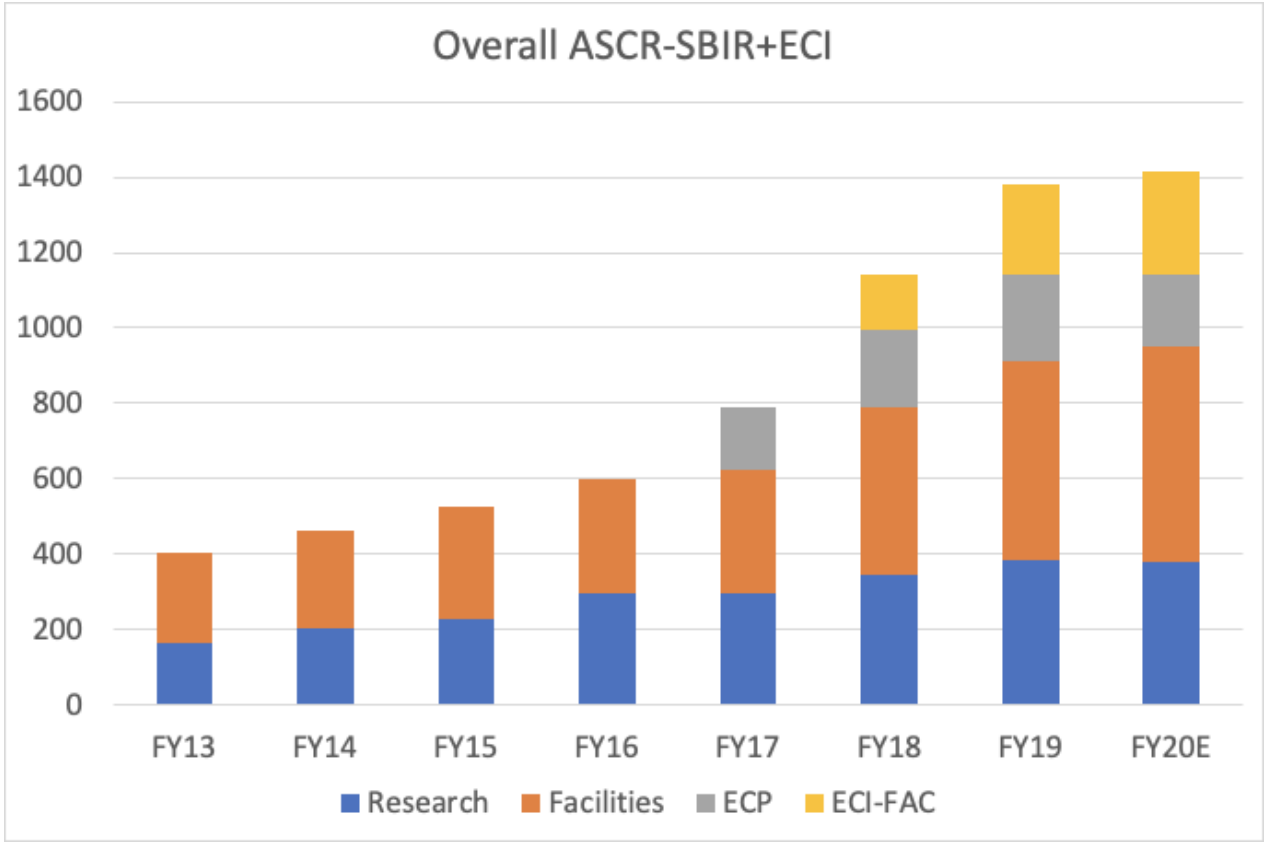
ASCR Budget over recent years

- ASCR/ASC have done a Big Wonderful Thing with ECP
- Big resources for the project
- Big strain on base resources before the project
- Post ECP:
  - “Big” ASCR ???
  - “Little” ASCR

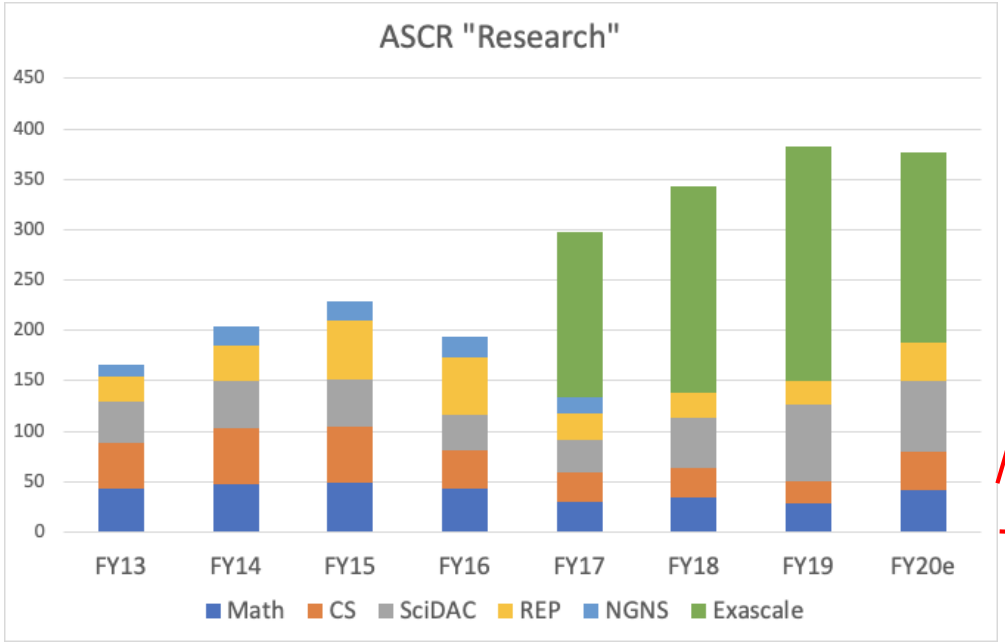
Depends on

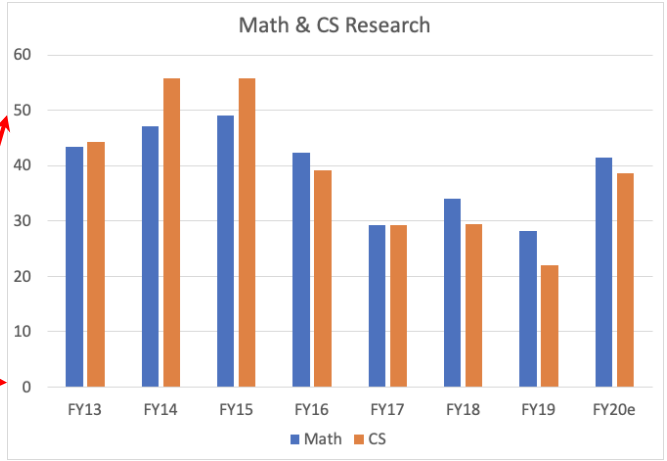
Mission Needs, Opportunities, Vision of Future

Total ASCR Budget FY13-FY20e



ASCR “Research” Budgets

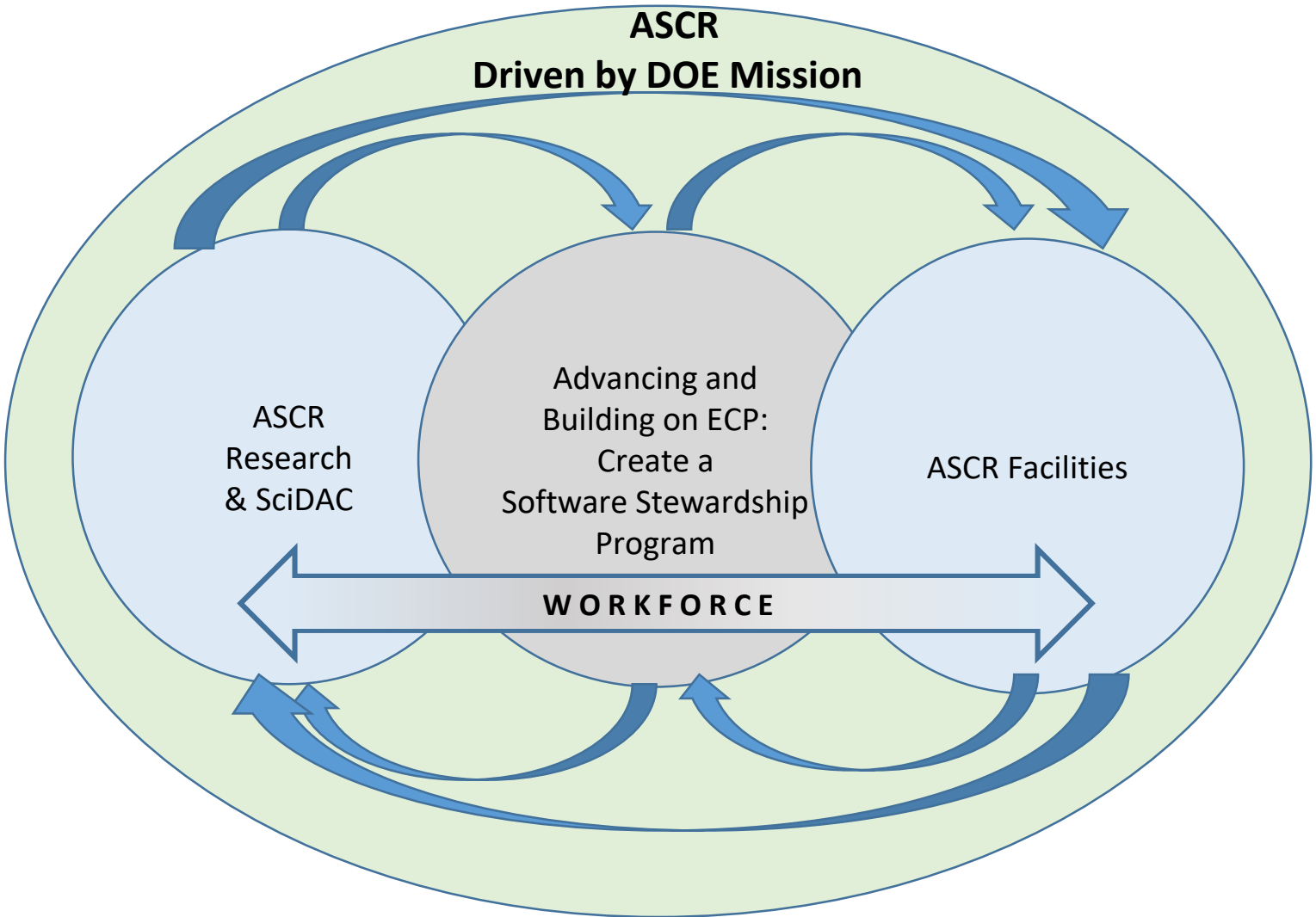




Transition

Findings and Recommendations Overview

- Advancing and Building on ECP:
  - Software Technology
  - Applications
  - Industry
  - Management
- Advancing ASCR Research
- Current and Future Workforce
- National and International Leadership


ASCR
Driven by DOE Mission
ASCR
Research
& SciDAC
Advancing and
Building on ECP:
Create a
Software Stewardship
Program
ASCR Facilities
WORKFORCE

A: Advancing and Building on ECP

Finding

A.1: ECP has been successful overall.

- Organizing unparalleled resources to design and develop exascale computing systems that will be deployed to satisfy DOE mission needs.
- Creating artifacts (computer systems, software libraries, demonstration applications)
- Modeling practices (in software engineering, management, co-design, collaboration among stakeholders) that should be expanded and built upon to realize the full impact of exascale computing.

Finding

A.2: ECP successfully managed a large distributed collaboration.

- Adapted rigorous project management requirements to large computer system development with co-design.
- Deep expertise and years of experience of the ECP L2 and L3 ST managers enormously valuable planning & development of the software ecosystem.
- Agile management practices, lightly integrated with EVM project management, is of great help in effective planning, coordination, and reactive modification of software technology (ST) R&D activities.

Finding

A.3: ECP Created a Software Ecosystem

- ECP has created a well-designed software ecosystem for development, curation, and distribution of exascale systems and application software.
- This ecosystem allows the integration of the fruits of years of basic research in mathematics and computer science into systems and applications.

Applications

- Collaborative Co-design: applications ⇒ heterogenous architectures.
- Deployment Pathway to ASCR Facilities.
- Integrated software ecosystem incorporating software products from years of prior ASCR and ASC research.
- Application Development (AD): 24 applications, 6 co-design centers, cross-platforms
- A culture of close interaction between AD and ST.
- Broad buy-in from senior management in DOE Office of Science and Applied Offices as well as NNSA.

System Software

- ~70 software products organized into 6 SDKs:
  (Programming models and Runtime; Compilers and Support; Tools and Technology; Math Libraries; Visualization Analysis and Reduction; and Data Management, I/O Services, and Checkpoint Restart).
- Dependence database
- Coordination of up to 8 Labs: software development, engineering, hardening for transition to facilities and applications.
- ST made effective use of modern software tools for collaboration, delivery/deployment integration and coordination: Atlassian, Spack, continuous integration, Git workflows, and containerization.
- The results had multiple software delivery vehicles: single products from source, SDK groupings for related products, and E4S for full suite installation.

Finding

A.4: ECP supported collaboration with Facilities and Industry

- ASCR and ECP/ECI have effectively collaborated with industry and the facilities to develop exascale computing technology and industry applications.
- Hardware and Integration (HI) and Facilities:
  - applications integration, resource utilization, hardware evaluation, PathForward, deployment of ECP software, training, and productivity.
- Culture of close interaction and coordination between AD and HI.
- The *xForward* programs
  - supported industry partners in technology development
  - successfully provided a shared context for industry and ECP hardware and software experts on the industry side to interact.
- ECP Industry Council: valuable perspectives on needs for world-class simulation and applications and facilities in the private sector and form interaction with national resources like the DOE labs.

Recommendation

A.1: Create a Shared-Software Stewardship Program within ASCR

ASCR should create a program to support and curate shared software based on the ECP ecosystem. This should incorporate ASCR program office oversight while delegating operational control to experts on the software engineering team.

Software Stewardship Vision

- Establish a DOE Shared Software Stewardship “hub” or “virtual laboratory” to **coordinate research, development and delivery** of DOE software products after the conclusion of ECP.
- Led by DOE laboratory and academic software leaders who possess long-term experience with DOE software development and delivery.
- Responsible for assessing and coordinating the evolution and growth of the ECP software stack, for developing advanced software packaging and delivery tools, and for keeping the software dependence database current/up-to-date.

Recommendation

A.2: Engage current and and anticipate future software needs

- Important software and algorithms can originate outside of DOE and ASCR.
- ASCR should continue to monitor and anticipate external developments in critical areas and incorporate this information in planning the evolution and modernization of software.
- This activity overlaps with but extends beyond the scope of the Stewardship program.

Recommendation

A.3: Collaborative Applications Support

- Transition ECP applications into SciDAC-like arrangements with joint funding from ASCR and application home organizations.
- Recompete as appropriate.

Recommendation

A.4: Broaden Industry and Academic Engagement

As new hardware and software technology needs are identified at the appropriate scale:

- the *xForward* model should be extended to hardware and independent software vendors to engage them early and substantively in new directions.
- Similar collaboration with university groups should be explored.

Recommendation

A.5: ASCR Program Management should adopt modern project management tools

- ASCR should adopt and incorporate modern project management tools into its programs to facilitate collaborative work between labs and programs.
- ECP has strong expert technical management embedded at many levels. We encourage ASCR to follow such a model for the programs and program managers that build on ECP.

Breathe...Discuss

NOTE: ECP Transition to Operations and Research Report

B: Advancing ASCR Research

Finding

B.1: Applied Mathematics and Computer Science Research is essential for future progress in advanced scientific computing.

- New fundamental Math and CS challenges:
  - new computing paradigms and devices.
  - Effective use of exascale class machines
  - Data challenges for instruments, edge computing with large dataflows
- Challenges are typically multidisciplinary.
- Exploratory R&D (high risk/high reward) is needed to enable fresh approaches.

Finding

B.2: ASCR's base research program has been constrained during ECP era.

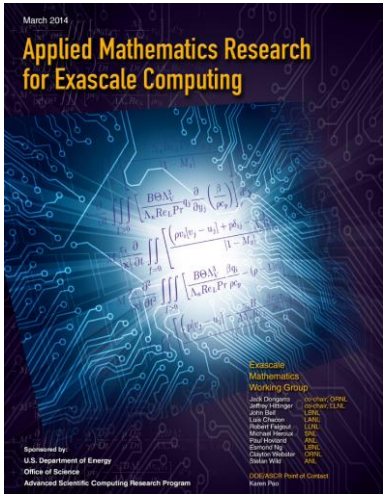
- Reinvigorating ASCR research is essential for the effective evolution and expansion of the ECP software ecosystem.
- The breadth of participation in ASCR research and ECP R&D was extremely constrained
  - participation was principally by the national labs and the project lost out on academic and industry contribution.

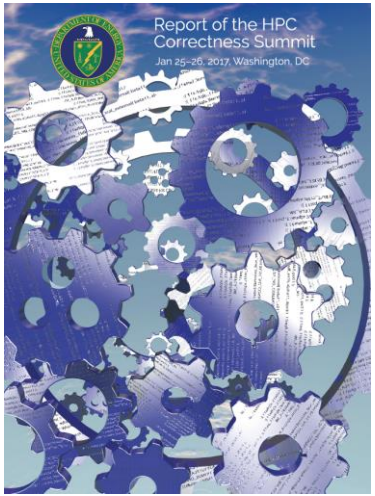
Recommendation

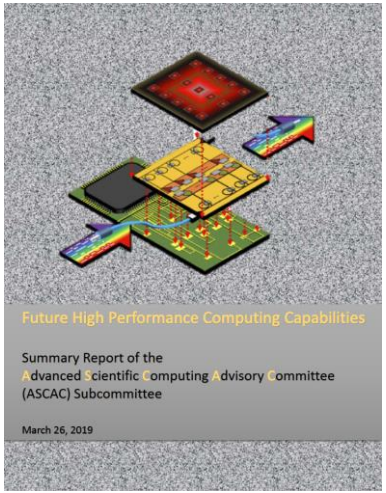
B.1: Substantially Reinvest in ASCR Research

- Significant expansion of the ASCR research investments in computer science and applied math
- The research program should encourage interdisciplinary work and appropriately scaled teams.
- Research funding opportunities should attract broad responses and appear at regularly predictable times.
- Exploratory R&D (high risk/high reward) is needed.

Research Directions...







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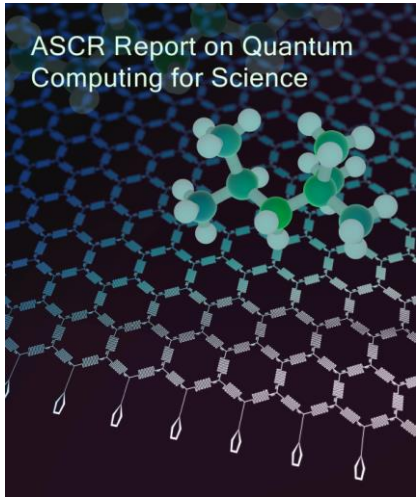

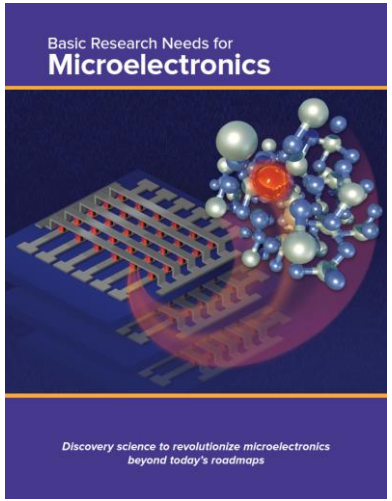

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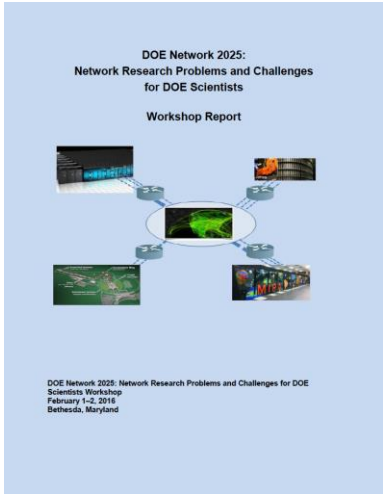
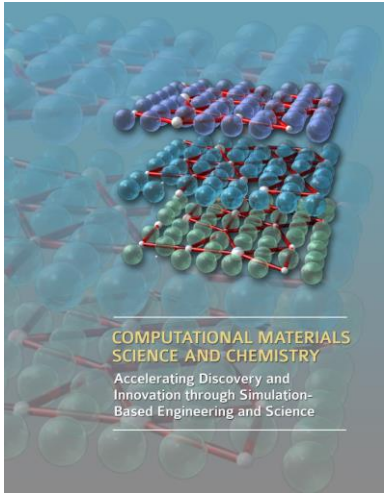
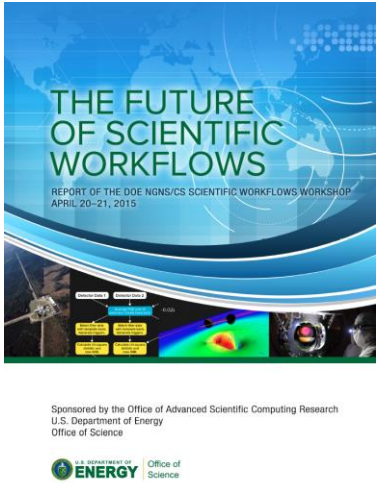






Recommendation

B.2: Renew a Stable Environment for Basic Research

Goal: a stable environment for long-term basic research.

- Reinvigorate DOE funding for basic research at DOE national laboratories and universities, and re-establish collaborative, interdisciplinary/multidisciplinary research.
- Include support for “blue sky” research which explores innovative, novel, and sometimes long shot ideas. This support should be accessible for investigators at all levels from early career to senior.

Recommendation

B.3: Distribute Research Software

Building on some of the ECP experience with “hardening” research software for wide reliable use, we recommend that ASCR create pathways to wider distribution and uptake of research results that make it to the threshold of distribution. This should be an ongoing continuous effort within the research programs.

Breathe...Discuss

Current and Future Workforce

Finding

C.1: A Skilled, Diverse, Motivated Workforce

During ECP there have been stellar examples of great work, but also challenges to the workforce pipeline at multiple stages.

- Built ties and trust between DOE/SC/ASCR communities, in large part through collaborative delivery of high-quality results.
- Extraordinary efforts at Facilities and Centers and Labs

Finding

C2: Career paths are challenged beyond Exascale

Outstanding Issues

- Career paths for both researchers and developers
- Retention of the talented workforce
- Diversity of the Lab workforce
- opportunities for blue-sky research as well as development.

Addressing workforce issues will be particularly critical during the transition to the post-ECP environment.

Finding

C3: Diversity, Equity, and Inclusion are valued.

- ASCR researchers value DEI, and are aligned with SC's efforts to increase DEI in the workforce
- Significant progress has been made during ECP and with SC leadership taking an active role supporting DEI
- Researchers at the Labs see multiple opportunities to improve DEI, which can be realized with appropriate support from leadership

Recommendation

C.1: Support researchers' re-engagement in "blue sky research"

ASCR should craft programs that develop a diverse multi-generational workforce.

Each career stage will have different needs and require different kinds of support.

- Early-career researchers will benefit from mentorship in building independent blue sky research programs, and support in building their professional networks for fulfilling research careers.
- Mid-career and senior researchers can expand their horizons and motivate their continued engagement during the transition.

Recommendation

C.2: Retain the Current Workforce

Researchers should understand they are valuable to the DOE mission during the transition and beyond. We recommend ASCR and ASC express this value.

- Attracting and retaining talented people requires that they feel **valued** as professionals, **connected** with their colleagues, **engaged** in contributing to the science mission goals of ASCR and DOE, and supported in their pursuit of career development opportunities.
- During transition, many researchers--especially those hired under ECP--will look to ASCR leadership for **indications about the future**, and their place in it. Stability? Opportunities for professional growth? How does my expertise fit?
- An **articulated vision** is essential for ASCR researchers to appreciate the opportunities to contribute during the transition and beyond.

Recommendation

C.3: Strengthen Ties to Universities and the Ecosystem

- Strengthen the talent pipeline, especially at the earliest stages
- Graduate students are next generation of researchers: Robustly fund University Research.
- Take advantage of the flexibility of staffing up research projects through universities and industry partners.
- Funding opportunities should arrive on a regular and predictable cadence. Funded awards should be administered predictably.

Recommendation

C.4: Create career paths for scientific software professionals

Many benefits of ECP have come from an increased focus on development.

Sustaining and growing the benefits of ECP will require the labs to recruit and retain world-class software developers.

In turn, this requires the labs to create suitable long-term career paths, comparable to those in industry.

Because these positions focus on delivering continued growth for ECP and ASCR products, they should sit with the ASCR research side rather than under facilities.

Recommendation

C.5: Support diversity, equity & inclusion (DEI)

A diverse workforce assures fresh perspectives and aspirations to achieve innovations targeted toward the breadth of national needs.

- SC is currently convening an external review of SC Lab DEI efforts, and ASCR should set ambitious goals based on the results
- Where feasible and appropriate, ASCR and the Labs's DEI efforts should take into account field-specific challenges in recruiting and retention
- ASCR should promote more family friendly work policies, mentoring, to specifically address women in the workforce and forms of diversity such as (but not limited to) ethnic diversity, LGBTQ, and people with varying abilities.

National and International Leadership

Finding

D.1: ECI/ECP is the leading national and international exascale computing effort.

As has happened throughout its history, DOE is pioneering the vision, design, creation, and application of the next incarnation of advanced scientific computing. When envisioned, the goal of developing exascale computing was advanced in SC/ASCR and NNSA/ASC and supported to meet the needs of DOE. As plans to design, invest in, and create exascale were formed, the consideration expanded to a national effort involving multiple agencies and stakeholders. It also help spawn exascale projects around the world.

Finding

D.2 New horizons in computing will impact DOE's mission.

DOE/ASCR must be prepared to work in a wider computing arena.

- ASCR naturally leads in some areas (eg, Advanced Sci Comp)
- Areas with opportunities for synergy between ASCR and peer leaders
- Areas the impact DOE mission where most development activities might be outside DOE/ASCR's domains

⇒ Judgment about where, how, and how deeply to engage.
⇒ Rich connections and interactions with a broad spectrum of interests..

Recommendation

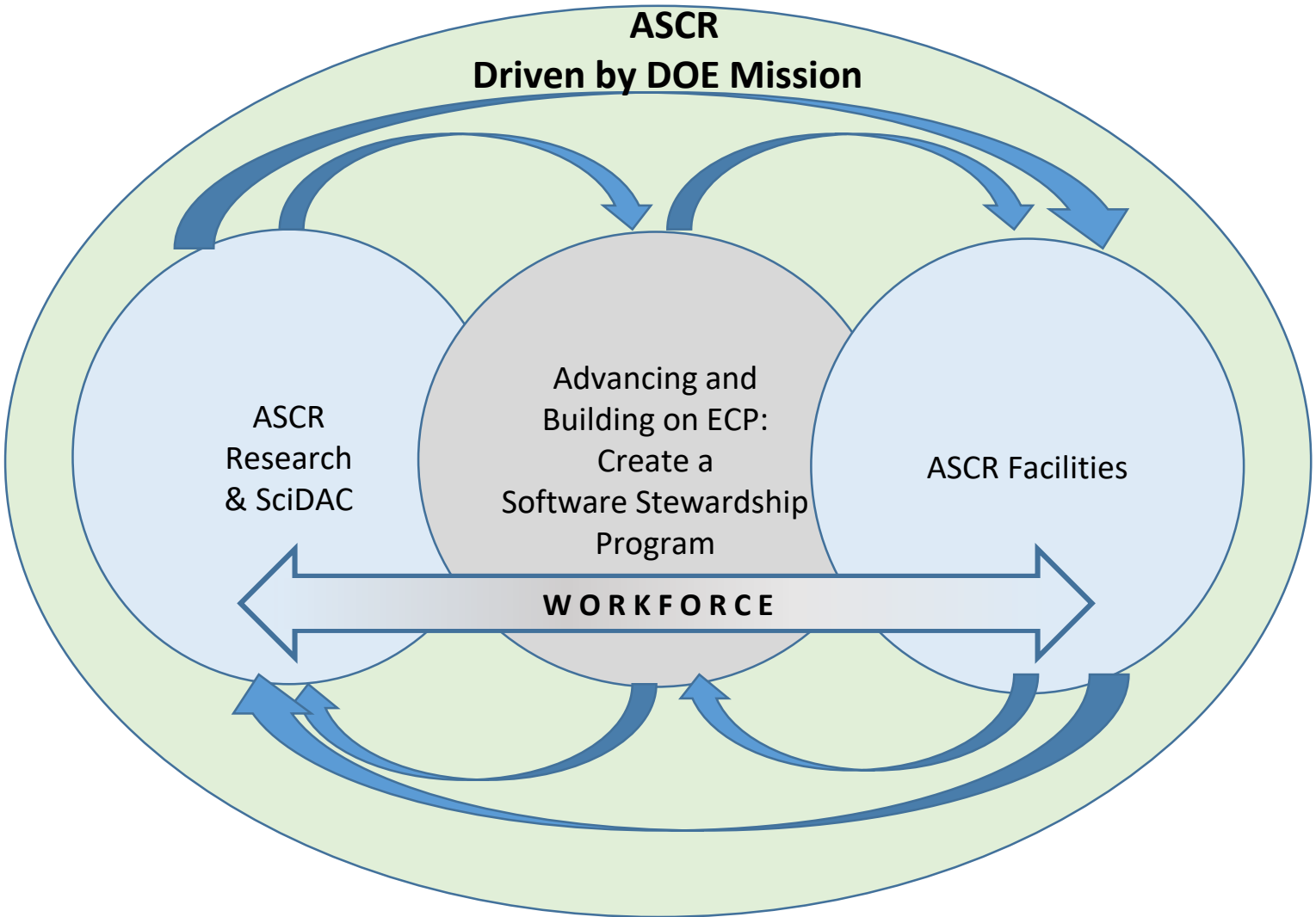
D.1: DOE/ASCR should maintain national and international leadership in advanced computing.

The recommendations we have made for the transition lay the foundation for ASCR research and ASCR technologies to impact future computing and DOE's mission. To maintain world leadership in scientific computing, DOE and ASCR need to be able to connect to stakeholders across US universities, industry, laboratories, and agencies.

Recommendation

D.2: ASCR programs should engage and collaborate with national stakeholders in other agencies.

ASCR should consider engagement strategies in new research areas such as AI and Quantum to leverage off of other agency efforts to further DOE mission.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Discussion

Thanks for your attention