

AUG 2024

ALCF-4 DESIGN REVIEW

EARLY SCIENCE PROGRAM



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ALCF Catalyst Team Lead

AGENDA



Times	Item	Owner
8:30	Executive Session	Review Chair
9:00	Welcome	Mike Papka
9:10	Project Overview	Jini Ramprakash
9:40	Technical Overview and Early Science	Kevin Harms Chris Knight
10:15	Break	
10:30	Technical Requirements	Taylor Childers
11:30	Benchmarks	Chris
12:15	(Working Lunch) Discussion & Questions from the committee	ALCF-4 Team
12:30	(Working Lunch) Executive Session	Review Chair
13:30	Facilities	Jon Cisek
14:15	ALCF-4 Risks Review	Noah / Jini
15:00	Break	
15:15	Executive Committee Q&A with ALCF-4 team	Review Chair
15:45	Executive Writing Session	Review Chair
17:00	Adjourn / Tour of Aurora	Susan Coghlan
18:00	Dinner	

CHARGE QUESTIONS

1. **Is the technical approach appropriate to support the ALCF-4 Mission Need requirements?**
2. Are the RFP technical requirements reasonable, clear, and consistent with the goals and objectives for the ALCF-4 project?
3. Does the ALCF facility upgrade plan support the system requirements specified in the RFP for the onsite options?
4. Have the major technical risks and appropriate mitigation strategies been correctly identified for this stage of the project?

ALCF EARLY SCIENCE PROGRAM

- Engaging and helping build a community to enable science on day 1
 - Dedicated staff and postdoc support for projects
 - Workshops, hackathons, webinars
 - Technical reports documenting computational efforts and lessons learned
- Successful Early Science Program (ESP) on deployed systems
 - ALCF-2: Mira
 - 16 projects working with ALCF postdocs/staff

<https://www.alcf.anl.gov/science/early-science-program>

<https://www.alcf.anl.gov/theta-early-science-program>

<https://www.alcf.anl.gov/mira-early-science-program>



ALCF EARLY SCIENCE PROGRAM

- Successful Early Science Program (ESP) on deployed systems
 - ALCF-3: Theta
 - 12 projects w/ support for 4 postdocs
 - ALCF-3: Aurora (ongoing)
 - 5 Simulation projects (originally 10)
 - 5 Data & 5 Learning projects (separate call for proposals in 2018)
 - Deep engagement between ALCF, COE, and ESP teams



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<https://www.alcf.anl.gov/mira-early-science-program>

ALCF EARLY SCIENCE PROGRAM OUTLINE

- Plan for Call for Proposals to open ~3 years before start of acceptance
- 12-15 projects selected competitively to span 3 pillars of Simulation, Data, and Learning
- Will continue ALCF practice of establishing a “Tools” ESP project to engage profiler and debugger developers

ALCF EARLY SCIENCE PROGRAM OUTLINE

- Desire to establish a “Software Technology” ESP project to engage software community
 - Provide a mechanism to engage with developers of libraries, abstraction layers, and other dependencies important to future workloads
 - Enables access to non-public resources similar to what the Exascale Computing Project enabled for Aurora
 - Possibly combine with “Tools” ESP project

- Ongoing discussions to potentially leverage an ESP project to enable broader engagement
 - Industry partners, ALCF Lighthouse Initiative, ...
 - Need will be influenced by expected availability of public “N-1” HW+SW

ALCF EARLY SCIENCE PROGRAM OUTLINE

- Key Performance Parameter (KPP)
 - INCITE-level computational readiness of projects
 - Effectively able to use >20% of the system
 - Leverage hardware for improved performance (e.g. GPUs)
 - Objective (75%) & threshold (50%), for example
 - EVMS method: BEI (Baseline Execution Index) using milestones
 - Quarterly milestones, same for all projects
 - Created annually, for subsequent year
 - Milestone reports are the deliverable for marking completion
 - Quarterly surveys on readiness metrics to track progress

ALCF EARLY SCIENCE PROGRAM OUTLINE

- ESP Project Support Model
 - Needed level of support impacted by multiple factors
 - Choice of vendor and system architecture
 - Application team readiness level
 - Adoption of new emerging software technologies, methods, and algorithms
 - Catalyst/POC at 30-50% FTE per project
 - Deep engagement, learn new HW+SW, develop best-practices

ALCF EARLY SCIENCE PROGRAM OUTLINE

- ESP Project Support Model
 - ALCF onsite postdoc per project
 - 3-year term
 - Considering 50% funded by ALCF-4, 50% funded by steady-state
 - Help ensure postdocs able to work on publishable research projects
 - Strong desire for all postdocs to complete their appointments after having accessed the full ALCF-4 system
 - Important for their career development (e.g. publications, presentations)
 - Vendor/COE POC per project (one person may support multiple projects)
 - NDA access to sequence of early hardware + software

ALCF EARLY SCIENCE PROGRAM OUTLINE

- Growing an ESP community
 - 1-on-1 interactions
 - Deep engagement of ALCF staff+postdocs, COE, and ESP teams
 - Hackathons
 - Multi-day events focused on single application or team
 - Engagement from multiple stakeholders: application team, ALCF, COE, Vendor, Tools, ST, ...



ALCF EARLY SCIENCE PROGRAM OUTLINE

- Growing an ESP community
 - Workshops
 - Multi-day events open to entire ESP program
 - Information sharing, making new connections, hands-on work
 - Applications Working Group
 - Periodic informal discussions open to entire ESP program (e.g. biweekly)
 - Opportunity to openly discuss progress, issues, solutions





ANY QUESTIONS?



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SUMMARY

- ALCF has taken a measured technical approach to the ALCF-4 project
 - Evaluate the market and available technologies
 - Engage with vendors on key issues relative to achieving performance goals within the project scope
 - Ensure ALCF applications software transition to ALCF-4 with appropriate support for software dependencies
 - Leverage successful ESP program to guide software transition
- Proceed with competitive procurement for ALCF-4 which allows for both on-premises cloud and new system sited at Argonne within the ALCF



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