Connecting Science with the DOE's Integrated Research Infrastructure

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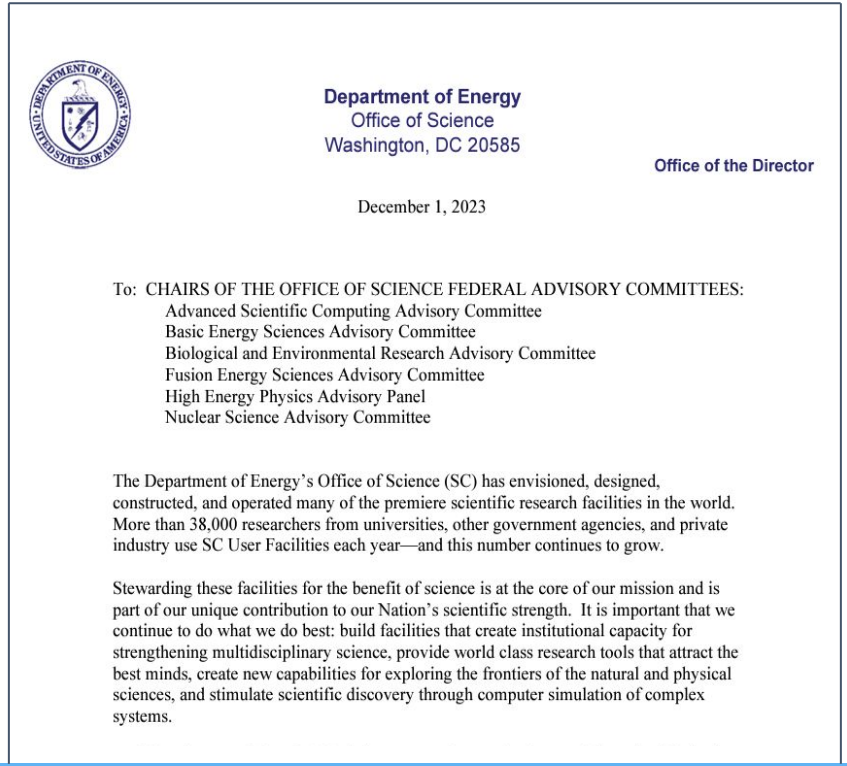
IRI Leadership Group

In December 2023, the SC Director charged the Office of Science to conduct an assessment of major projects within the Office

The Chairs of the SC Federal Advisory Committees were asked to "look toward the scientific horizon and identify what new or upgraded facilities will best serve our needs in the next ten years (2024-2034)."

This charge was only the third time the Office of Science (SC) conducted an SC-wide projects assessment.



Department of Energy
Office of Science
Washington, DC 20585

Office of the Director

December 1, 2023

To: CHAIRS OF THE OFFICE OF SCIENCE FEDERAL ADVISORY COMMITTEES:
Advanced Scientific Computing Advisory Committee
Basic Energy Sciences Advisory Committee
Biological and Environmental Research Advisory Committee
Fusion Energy Sciences Advisory Committee
High Energy Physics Advisory Panel
Nuclear Science Advisory Committee

The Department of Energy's Office of Science (SC) has envisioned, designed, constructed, and operated many of the premiere scientific research facilities in the world. More than 38,000 researchers from universities, other government agencies, and private industry use SC User Facilities each year—and this number continues to grow.

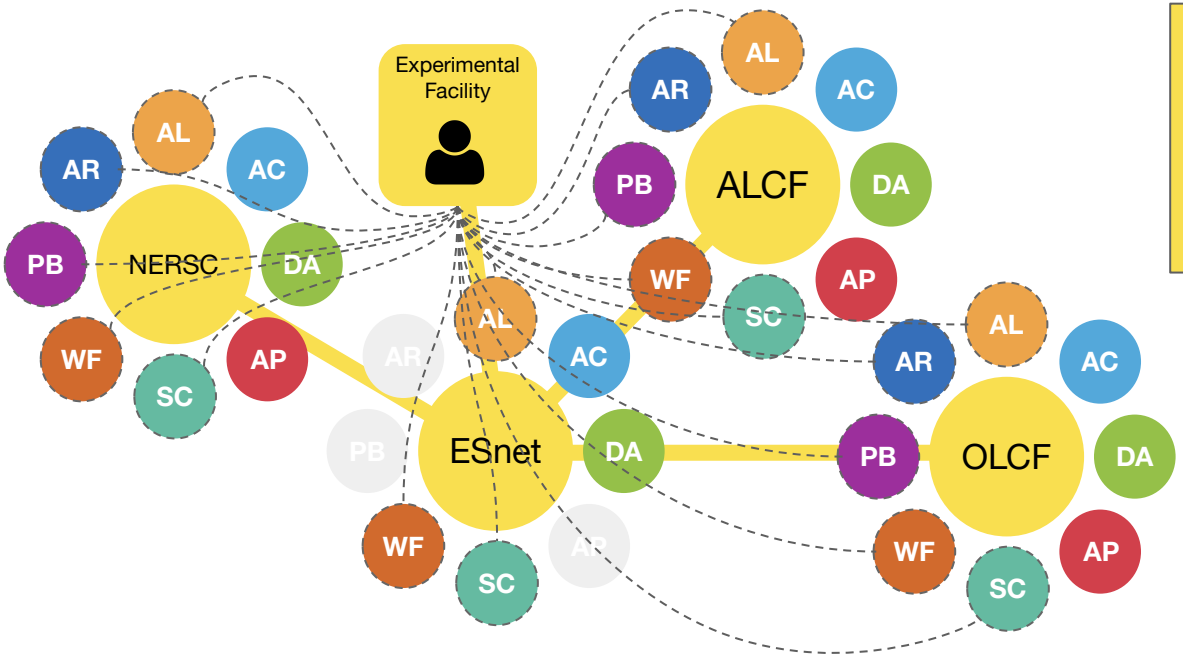
Stewarding these facilities for the benefit of science is at the core of our mission and is part of our unique contribution to our Nation's scientific strength. It is important that we continue to do what we do best: build facilities that create institutional capacity for strengthening multidisciplinary science, provide world class research tools that attract the best minds, create new capabilities for exploring the frontiers of the natural and physical sciences, and stimulate scientific discovery through computer simulation of complex systems.

The ASCAC Facilities charge report emphasized the importance of an integrated facility ecosystem for DOE science

Recommendation 2: Science demands integration. We advocate viewing ASCR facilities not as isolated entities, but as integral components of a single, larger integrated computational *ecosystem*…, with a single governance model.

… Further, this integrated ecosystem is required for programs of other agencies, and industry. Its critical role in bolstering national scientific and technological capabilities, as well as its status as a model internationally, cannot be overstated.

In an Integrated Research Infrastructure, simple things should be simple, and complex things should be possible



Today, an experimental facility must arrange separate bespoke interactions with individual HPC/HPN facilities.

AL	Allocations	SC	Scheduling
AC	Accounts	WF	Workflows
DA	Data	PB	Publication
AP	Applications	AR	Archiving

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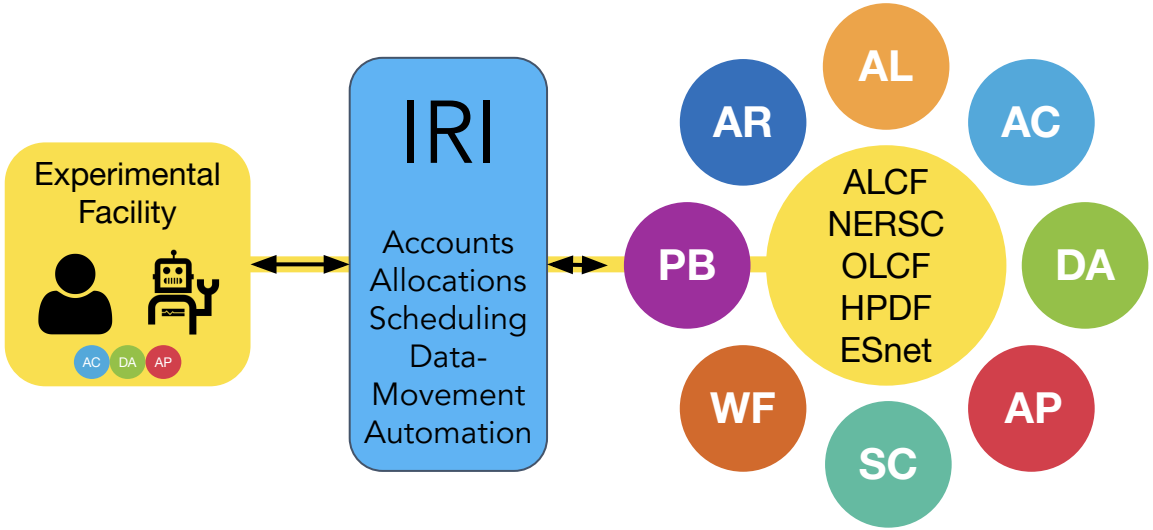

An IRI paradigm with common interfaces could simplify integration of an experimental facility with multiple HPC/HPN facilities.

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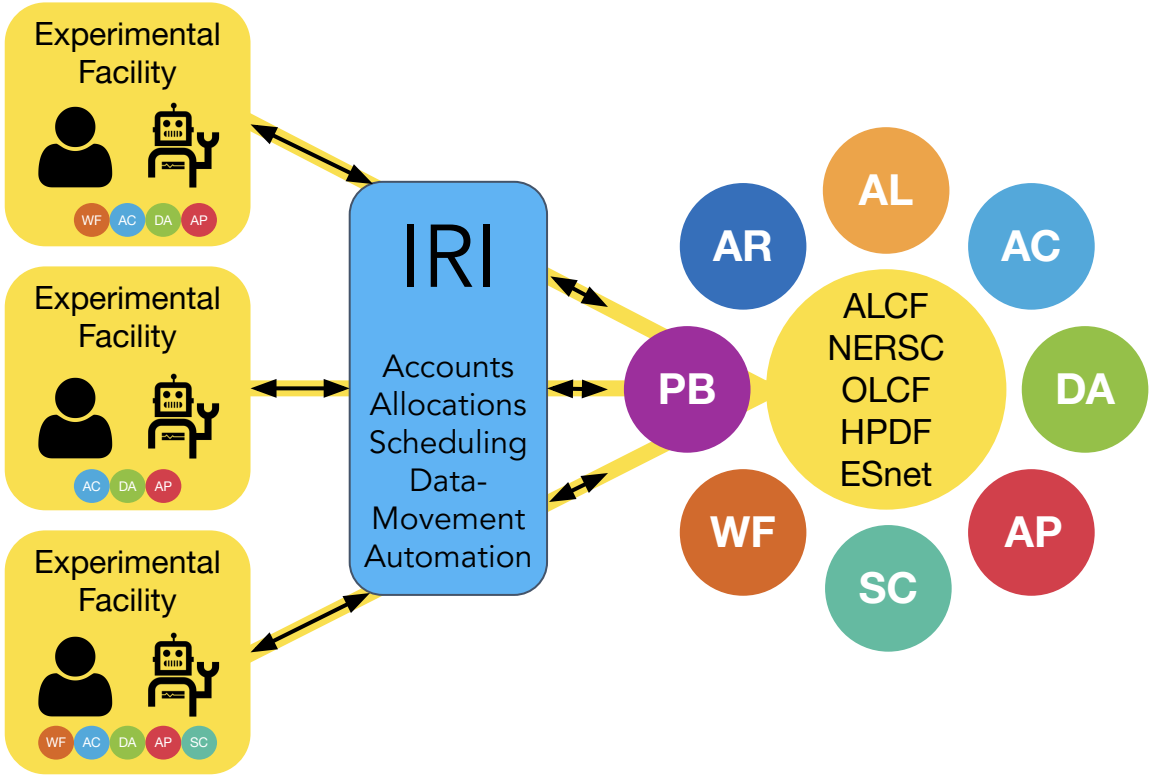

These common interfaces could support expansion and integration across multiple experimental facilities and HPC/HPN facilities.

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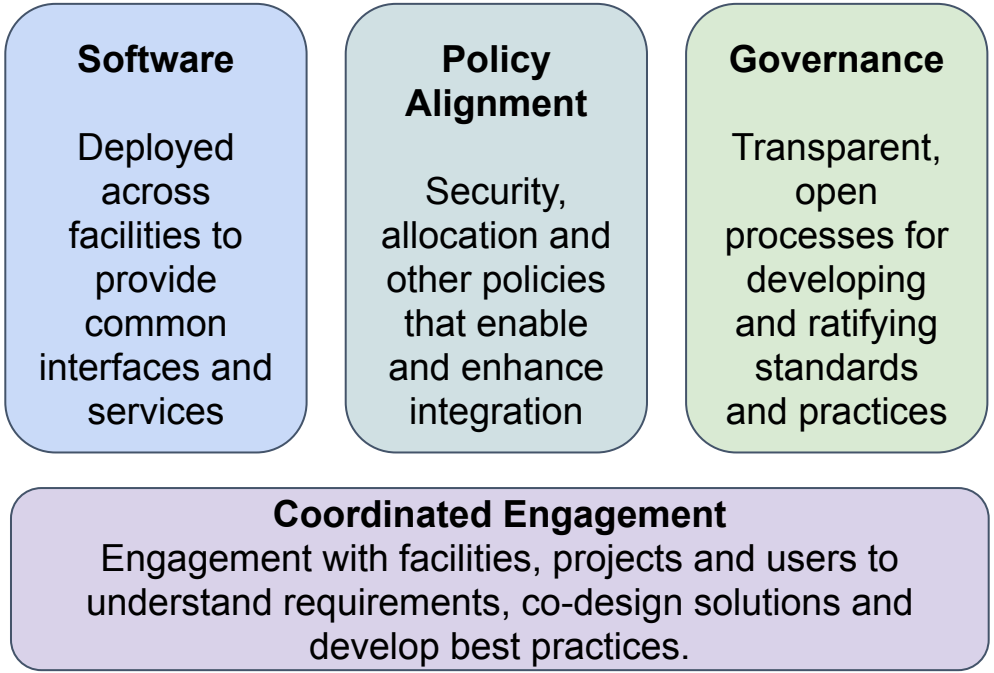
IRI is creating the OS for the DOE Ecosystem

IRI is an "operating system" that layers on top of existing facilities.

Facilities will need to make changes to support IRI software, policies and processes, but IRI does not dictate the physical hardware to be deployed at each site. Facilities retain their unique mission and capabilities.



IRI is creating the OS for the DOE Ecosystem

IRI is a **program** across all ASCR Facilities, other DOE user facilities, and participating Domain partners.

The IRI program involves the whole ASCR Facilities ecosystem (and potentially, the broader research computing ecosystem).

Software

Deployed across facilities to provide common interfaces and services

Policy Alignment

Security, allocation and other policies that enable and enhance integration

Governance

Transparent, open processes for developing and ratifying standards and practices

Coordinated Engagement

Engagement with facilities, projects and users to understand requirements, co-design solutions and develop best practices.

IRI has been developing over the past 5 years. The program launched this year.

FY 2021 President's Budget Request includes **Integrated** Computation and Data Infrastructure Initiative

ASCR IRI Task Force launch

ASCR IRI Task Force report

SC IRI Blueprint Activity launch

IRI Blueprint Activity results

FY 2024 PBR advances IRI and the High Performance Data Facility

HPDF Selection

GO

IRI Program Development

Jan **2020** Jan **2021** Jan **2022** Jan **2023** Jan **2024**

Vision **Strategy** **Implement**

The IRI Architectural Blueprint Activity collated and categorized the many challenges scientists face in building workflows integrated across DOE resources.

The IRI Framework comprises:

> 3 IRI Science Patterns represent integrated science use cases across DOE science domains.

Time-Sensitive Patterns	Data-Integration Patterns	Long Campaign Patterns

> 6 IRI Practice Areas represent critical topics that require close coordination to realize and sustain a thriving IRI ecosystem across DOE institutions.

Workflows, Interfaces & Automation	Scientific Data Lifecycle	User Experience
Cybersecurity & Federated Access	Portable/Scalable Solutions	Resource Co-Operations

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- User Experience
- Cybersecurity & Federated Access
- Portable/Scalable Solutions
- Resource Co-Operations

IRI is now implementing the frameworks proposed in the ABA

IRI Program launch is a DOE FY24-25 Agency Priority Goal
ASCR is implementing IRI through these four major elements

1 Invest in IRI foundational infrastructure

ASCR Facilities are architected to support IRI

- KPPs, benchmarks and readiness programs are explicitly designed for IRI

2 Stand up the IRI Program governance and technical activities

The IRI Management council has been established, and is working to:

- Define roles, responsibilities and reporting structures
- Launch committees to coordinate technical and outreach work

3 Bring IRI projects into formal coordination

We are coordinating existing work and forging new collaborations

- Roadmap for partnering with science teams
- Coordinating with CS research programs

These are each essential.
These are all connected.

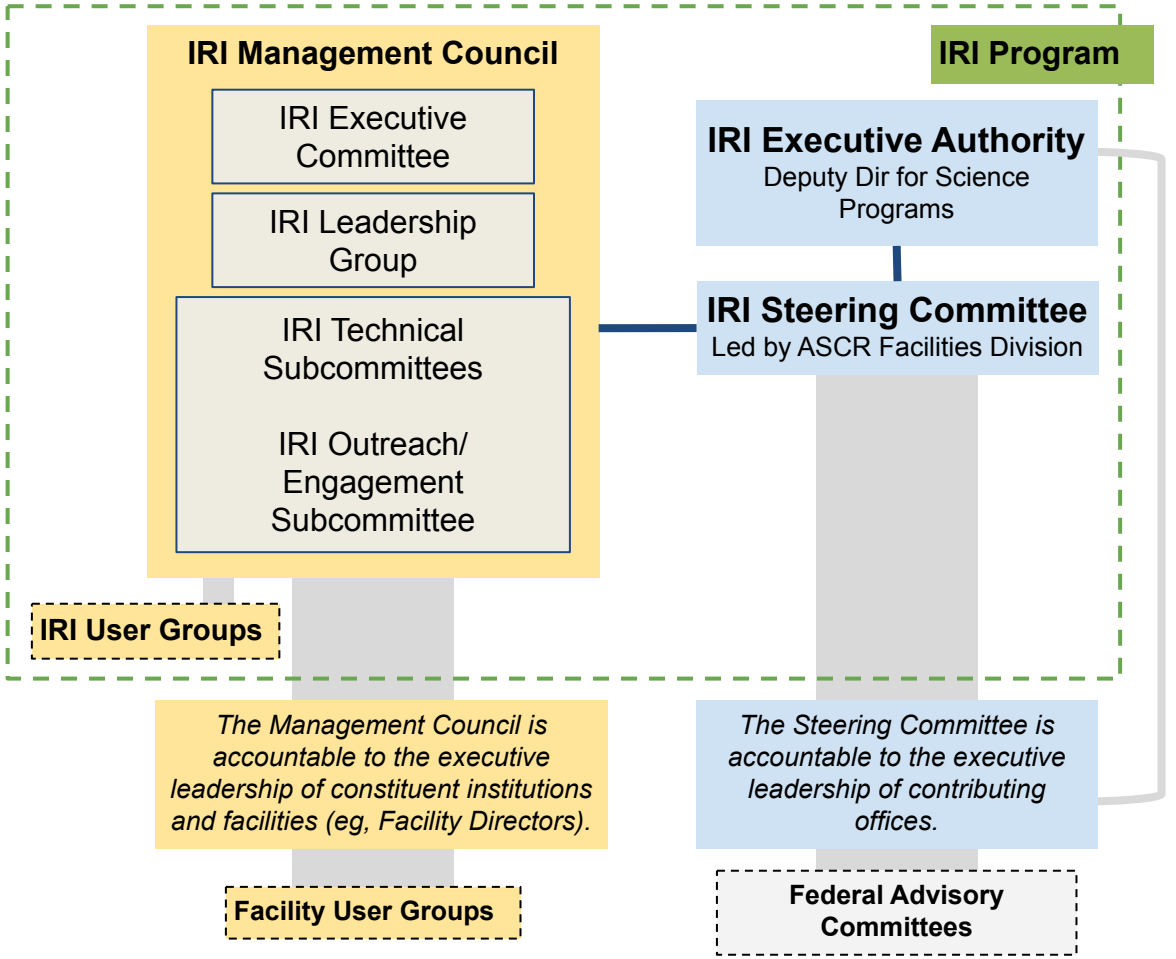
4 Deploy an IRI Science Testbed across the ASCR Facilities

Shared development environment for IRI developers and pilot applications, designed to accelerate transition to operations

The IRI Governance model

This structure was developed by the SC Headquarters IRI Coordination Group in 2022-23.

In late 2023, ASCR directed the ASCR Facilities to jumpstart the IRI Management Council.



Initial IRI program areas are drawn from the ABA Practice Areas

IRI-ABA Practice Area	IRI Program Area	Status
Resource Co-Operations	IRI Allocations Program Scheduling/Preemption Technical Subcommittee	Under development Under development
Cybersecurity and Federated Access	TRUSTID Technical Subcommittee	Launched!
User Experience	Outreach/Engagement Technical Subcommittee	Launched!
Workflows, Interfaces & Automation	Interfaces Technical Subcommittee	Launched!
Scientific Data Lifecycle	Data Movement Technical Subcommittee	Under development
Portable / Scalable Solutions	Software Deployment and Portability	Under development

IRI technical work will be managed via Technical Subcommittees

Their role is to identify goals and coordinate work in a particular technical area.

Launched May 2024

Outreach & Engagement Technical Subcommittee

- **Liaise with Pathfinder partners** to help demonstrate cross-facility workflows using early IRI frameworks
  - Coordinate work between Pathfinder teams and IRI
  - Identify and develop requirements and requirements strategy
- Develop and execute a plan for **broader community engagement**

Co-chairs: Eli Dart and Rafael Ferreira Da Silva
Members: Johannes Blaschke, Dale Carder, Jack Deslippe, Drew Paine, David Rogers, Katherine Riley, Tom Uram

Launched May 2024

Trusted IRI Designs (TRUSTID) Technical Subcommittee

- Define federated ID **design patterns** to enable trusted interoperable cross-facility workflows within the IRI ecosystem
- Promote **interoperability** and use of existing standards
- Create documentation, best practices, and **reference implementations**

Convened by Carol Hawk
Co-chairs: Ryan Adamson and Tiffany Connors
Members: Bill Allcock, Carl Bai, Scott Campbell, Maxim Kowalski, Jeff Neel, John Riney, Adam Slagell, Veronica Vergara

Launched May 2024

Interfaces Technical Subcommittee

- Design a **minimal functional API** and deploy it at multiple sites
  - Review existing API schemas
  - Propose IRI schema: endpoints, architecture, infrastructure,...
  - Implement MVP
- Explore how to align **Jupyter** across sites

Co-chairs: John MacAuley and Ryan Prout
Members: Bill Allcock, Ilya Baldin, Bjoern Enders, Paul Rich, Addi Thakur, Gabor Torok, Xi Yang

Pathfinder Projects - "It takes a village …."

The IRI program has identified "pathfinder projects", nominated by their program managers as ready to partner with us in the first stages of developing IRI technologies. Pathfinders will partner closely with IRI to:

- Facilitate collaborative co-design to leverage expertise across multiple disciplines
- Demonstrate feasibility to validate initial ideas and technical capabilities
- Promote knowledge sharing to accelerate paths to solutions

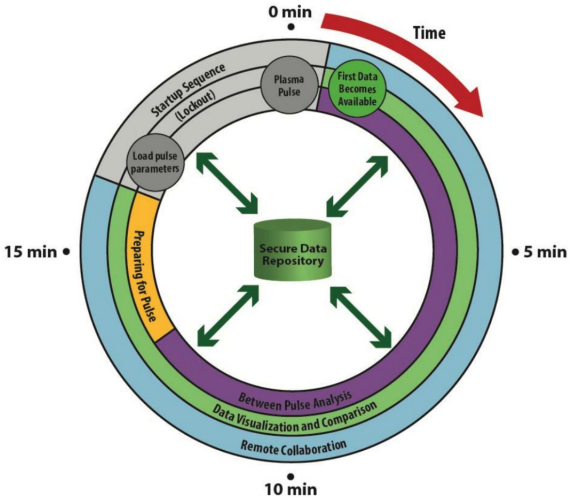
DIII-D

ESGF

BES Light Sources

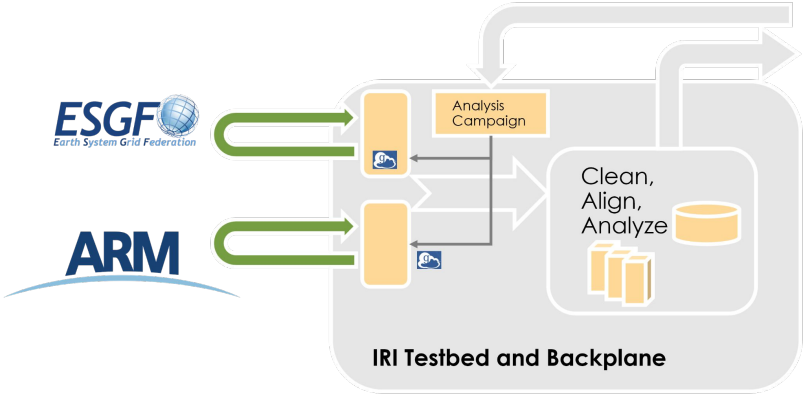
DIII-D pathfinder project

- The DIII-D fusion science team need to make decisions about how to tune their experiment parameters between plasma shots.
  - Working towards a computing model for ITER, which will produce 1PB/day
- DIII-D is partnering with ALCF, ESnet, and NERSC to run analyses robustly during experiments.
- **IRI goal**: DIII-D will have automated, resilient, fast turnaround for large-scale data analysis coupled with simulation ("digital twin").



ESGF Pathfinder project

- The Earth System Grid Federation (ESGF) provides access to world's largest climate model data archive
  - Growing multi-PB archive across the labs and worldwide
  - Thousands of scientists leverage climate data in their research.
- The ESGF2-US project is collaborating with ALCF, OLCF and Globus to support cross facility workflows
- **IRI goal**: ESGF will have resilient computing and distributed data services to make the archive more accessible to a broader set of users.



User-facing value added products accessed through
- Notebooks
- Viz tools
- Portals

BES Light Sources Pathfinder projects

- The BES light sources need a scalable and adaptive end-to-end architecture for data management and compute to accelerate time to science
  - Multiple order-of-magnitude increase in demand for computing resources over the next decade
- APS, ALS, LCLS and NSLS-II are collaborating with ALCF, ESnet, NERSC, and OLCF to demonstrate multi-facility resource coordination
- **IRI goal**: BES light sources will have access to a multi-tiered architecture with varying types and scales of computing, networking, and storage capabilities.

ALS ADVANCED LIGHT SOURCE

NSLS-II

Advanced Photon Source

DIII-D

LCLS

ESGF2 US

Pathfinder Projects

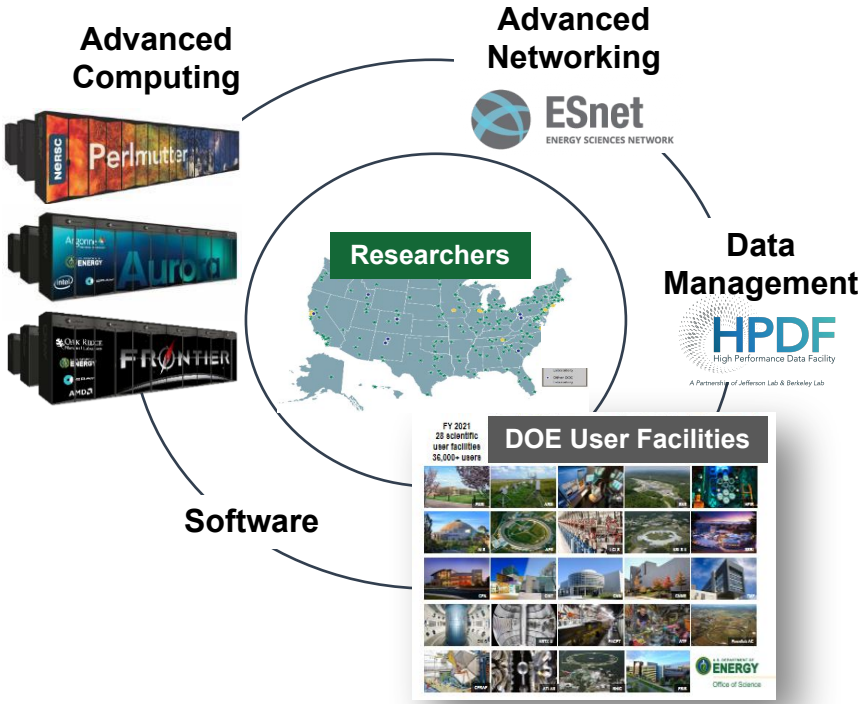
NP	Large-scale simulations integrating experimental data from DOE and international nuclear physics facilities.
NP	AI/ML incorporated into simulations to drive exploration of parameter space using codes like LAMMPS in the workflow.
NP	GRETA spectrometer online computing pipeline construction - for 1-5 day campaigns.
HEP	Astronomical spectroscopic observations at DESI/KPNO, survey data daily streaming to HPC, target selection pipeline.
HEP	Astronomy data management - DESI workflows - processing 100s of TBs of data utilizing HPC.
HEP	LHC simulation workflows; event generation for integration of WLCG with HPC.
HEP	Event generation for of complex simulation pipeline. Distributed, compute-intensive but not data-intensive.
FES	Heterogeneous data handling and real-time analysis for fusion power experiment steering at DIII-D and JET for fusion.
FES	DIII-D Fusion experiments + simulations, near-real-time analysis to determine/predict plasma conditions.
FES	DIII-D Tokamak plasma physics experiments - diagnostic data collection.
FES	Fusion workflows: 10s ~45GB per pulse, about 500TB total using custom SQL and NoSQL databases, computing with local and institutional resources, data exposed via APIs also for future ITER workflows.
FES	Data management and real-time analysis for fusion experiments at PPPL.
BES	Beamline data transfer at scale to HPC for real-time analysis and experiment steering, data transfer at scale to HPC (e.g., at SSRL).
BES	Metallurgy, MIDAS x-ray analysis software for APS high-energy X-ray diffraction microscopy beamline data. High data throughput. Pipeline development to NERSC and ALCF for on-demand computing at scale.
BES	Autonomous AI/ML-driven experiments such as for ALS and NSLS-II.
BES	APS 8-ID-I Smal-angle XPCS x-ray spectroscopy, high-frame rate camera, data management workflow including HPC. 0.2 PB of unsparsified data generated/day.
BES	Materials science. High data throughput, facility data transfer from APS to PNNL for analysis.
BES	Light source data processing workflows for large datasets (TBs to PBs), particularly ptychography; using AI/ML to help reduce data quickly.
BES	Data pipelines for high-speed detectors used at lights sources and NSRCs. Workflow development using NERSC.
BES	ML Autonomous materials characterization workflows using data (100s GBs per day) collected at light sources, neutron sources, and NSRCs.
BER	Combining multi-modal data from simulations and experiments for molecular scale imaging workflows (instrument + compute + storage).
BER	Crystallography microscopy and synchrotron light sources workflows and local and HPC computing.
BER	HPC-enabled high throughput sequencing, large scale sequence data analysis, sample and data life cycle, data product development (e.g., at JGI).
BER	Applying AI/ML to EMSL data for analysis.

Architecture Blueprint Activity

IRI technical work is driven by the Architecture Blueprint activities, requirements from Pathfinder projects, **and** many collaborations with science teams doing IRI-relevant work.

The ASCR Facilities are firmly embedded in the IRI ecosystem

IRI is permeating everything we do. **Multi-facility workflows** are an integral part of our major infrastructure design and strategic planning.



- IRI requires an exponentially growing amount of collaboration across ASCR facilities - it's changing how we work together
- ASCR facilities have made a lot of progress in supporting complex workflows
- Ongoing projects, testbeds, and major acquisitions are targeting IRI (ESnet6, NERSC-10, OLCF-6, HPDF and ALCF-4)

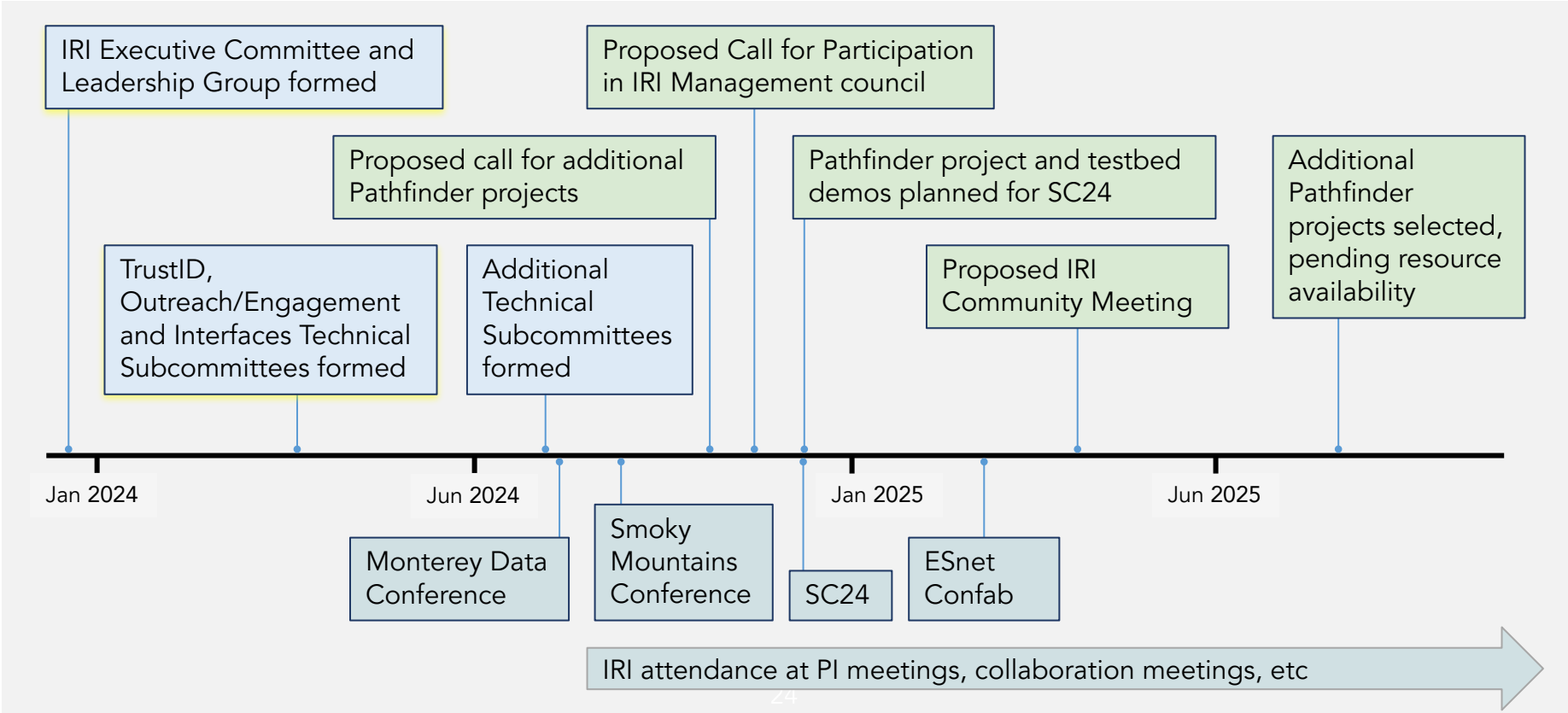
IRI will provide a foundational infrastructure for next-generational experimental science, post-exascale computing, AI/FASST* and other initiatives.

The IRI program is moving out of the initial stages of development and process-setting

- Launching first phases of science engagements and technical work
- Building organizational structure to manage IRI efforts and integrate across program offices
- Connecting to research programs
- Developing partnerships with pathfinders, and laying out the pathways to engage more broadly

**Frontiers in Artificial Intelligence for Science, Security and Technology (FASST) <https://www.energy.gov/fasst>*

IRI is moving!



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