OAK RIDGE National Laboratory | LEADERSHIP COMPUTING FACILITY

Bridging **Traditional Science** and **Autonomous Laboratories** Through **Integrated Research Infrastructure** and **Intelligent Workflows**

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U.S. DEPARTMENT OF ENERGY

ORNL IS MANAGED BY UT-BATTELLE LLC
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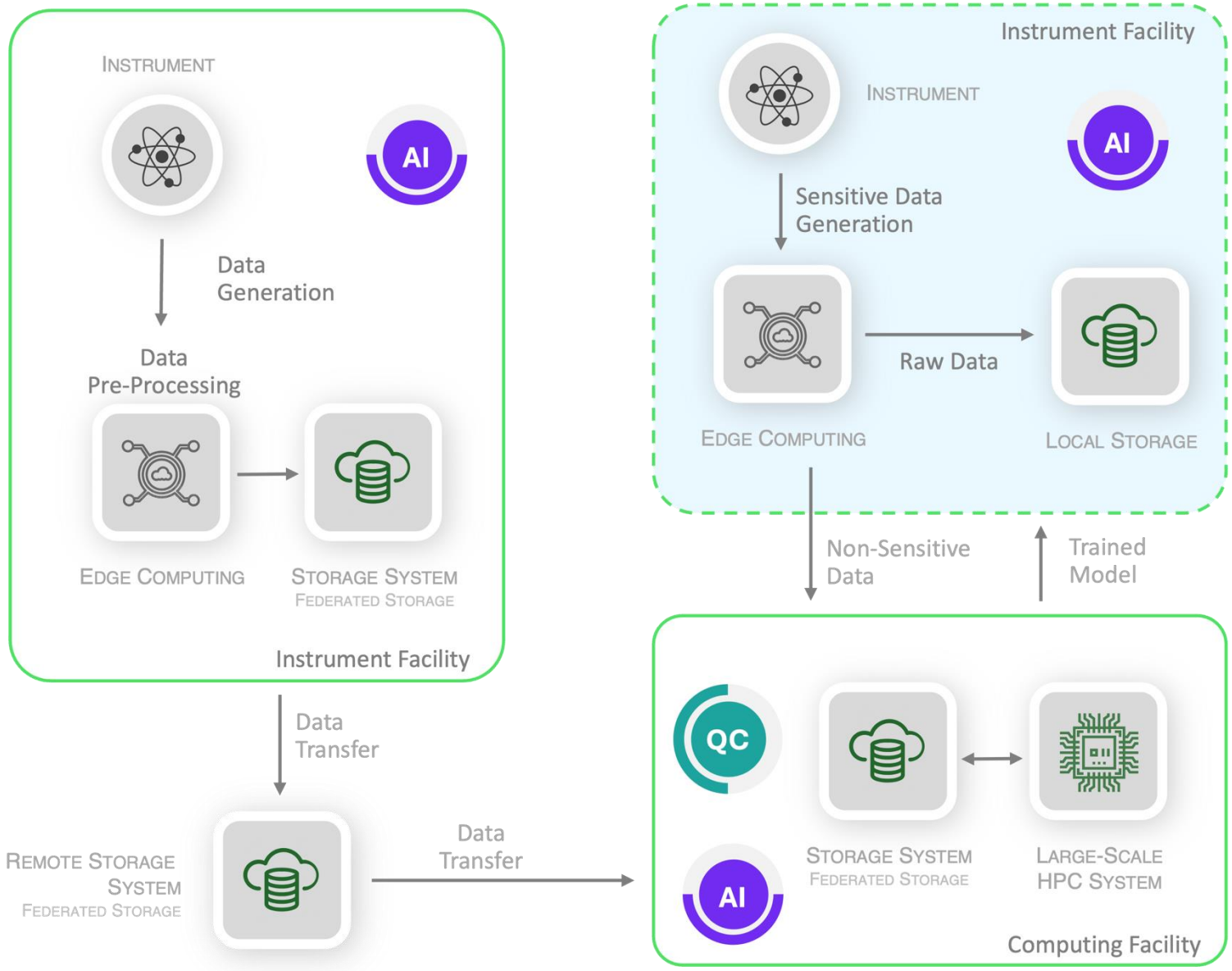
The Now

CURRENT STATE: MANUAL
ORCHESTRATION ACROSS FACILITIES

GROWING COMPLEXITY:
AI/ML + HPC + QUANTUM



The Future

INTEGRATING DIVERSE COMPUTING PARADIGMS

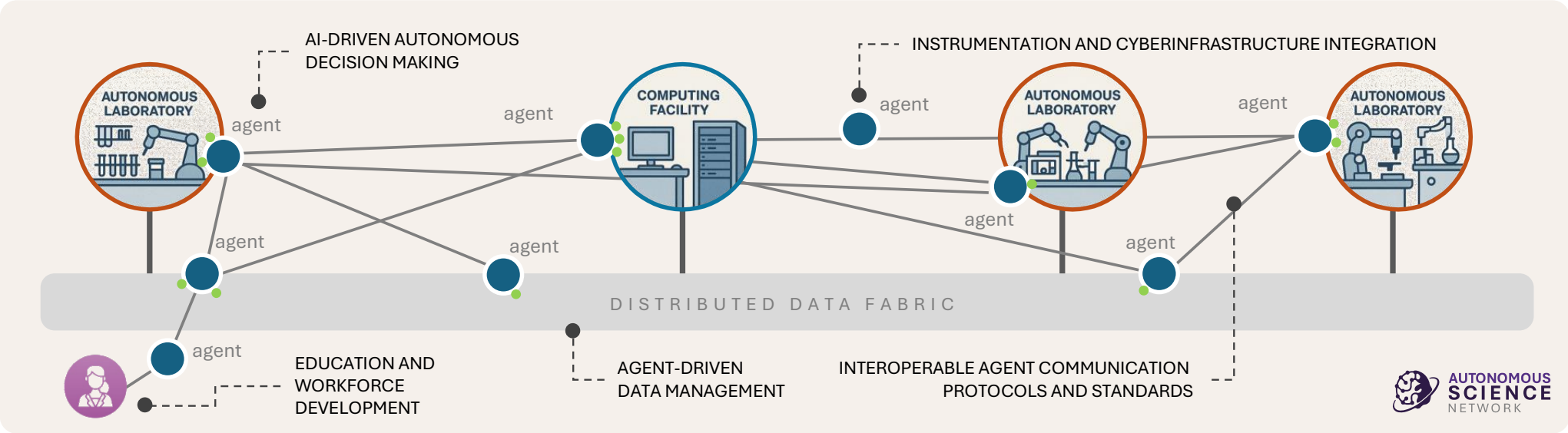
- **HPC + AI/ML + Quantum** working in harmony
- Seamless resource sharing across facilities
- Automated **workflow optimization and steering**

KEY TRANSFORMATIONS

- From manual orchestration to **autonomous operation**
- From single-facility to distributed execution
- From batch processing to **near real-time response**

CRITICAL NEEDS

- **Standardized protocols** for cross-facility integration
- **Dynamic resource management** for hybrid workflows
- Unified authentication and data movement standards



Next-Generation Scientific Labs

INTEGRATE AI WITH SCIENTIFIC METHOD

- Develop **hybrid AI systems** that combine data-driven learning with scientific principles
- Address critical **timescale mismatch** between **human and machine operations**

BUILD CONNECTED INFRASTRUCTURE

- Establish standardized **cross-facility protocols** for data and authentication
- Create **sustainable ecosystems** spanning instruments and computing systems

ENSURE SCIENTIFIC RIGOR

- Transform **workforce development** by integrating AI/ML with domain expertise
- Maintain essential **human insight** while leveraging automation

Shaping the Future of Self-Driving Autonomous Laboratories Workshop

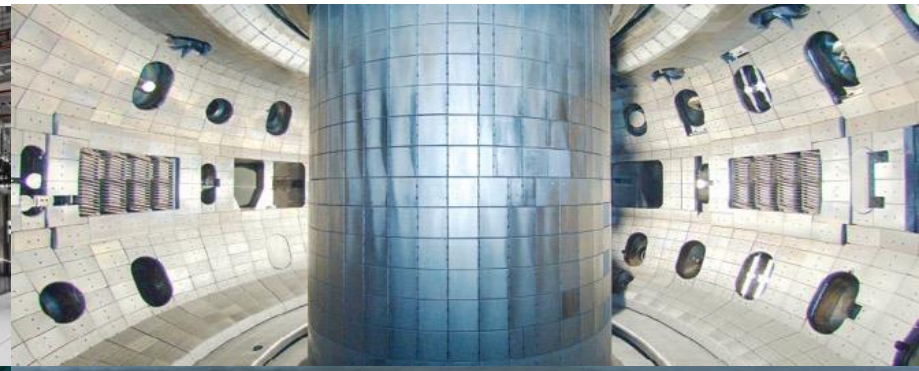
Workshop Report – November 7-8, 2024

https://doi.org/10.5281/zenodo.14588062

DOE User Facilities

Linking DISTRIBUTED RESOURCES is becoming paramount
to modern collaborative science, to integrated science

The challenges of our time call upon DOE and its national laboratories to be an OPEN INNOVATION ECOSYSTEM



DOE's Integrated Research Infrastructure Blueprint Activity

The key organizing elements of the IRI Framework are Science Patterns and Practice Areas:

IRI Science Patterns that represent integrated science use cases across DOE science domains and

IRI Practice Areas that will support the realization of a DOE-integrated IRI ecosystem

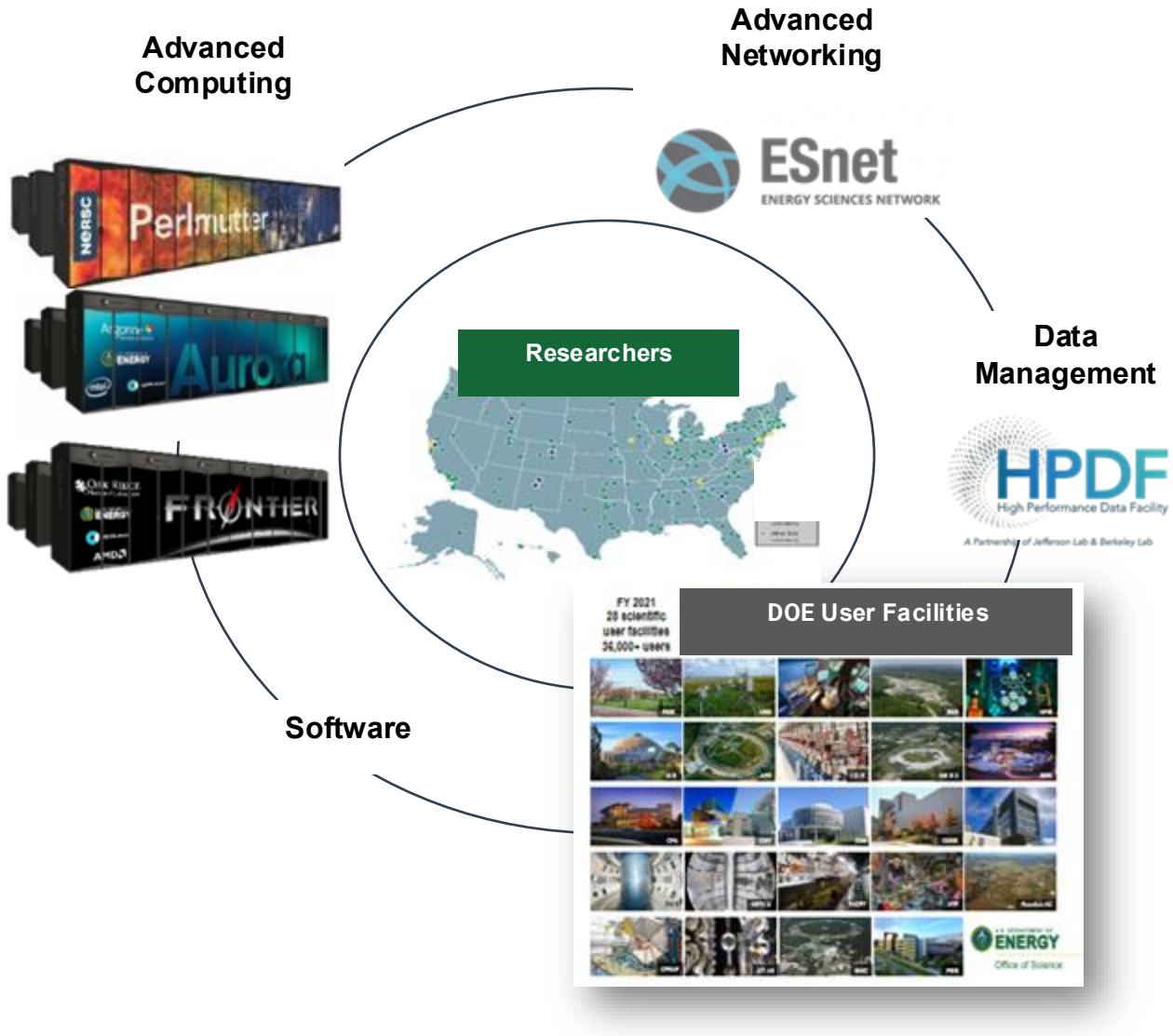
https://www.osti.gov/biblio/1984466

Convened over **150 DOE national laboratory experts** from **all 28 SC user facilities** across **13 national laboratories** to consider the **technological, policy, and sociological challenges** to implementing IRI

DOE's IRI Program

To empower researchers to meld DOE's world-class research tools, infrastructure, and user facilities SEAMLESSLY and SECURELY in novel ways to radically ACCELERATE DISCOVERY and INNOVATION

IRI is permeating everything we do – MULTI-FACILITY WORKFLOWS are an integral part of our major infrastructure design and strategic planning



Integrated Research Infrastructure Program

https://iri.science

A Framework for IRI Implementation

IRI SCIENCE PATTERNS

TIME-SENSITIVE PATTERN has urgency, requiring real-time or end-to-end performance with high reliability, e.g., for timely decision-making, experiment steering, and virtual proximity

DATA INTEGRATION-INTENSIVE pattern requires combining and analyzing data from multiple sources, e.g., sites, experiments, and/or computational runs

LONG-TERM CAMPAIGN pattern requires sustained access to resources over a long period to accomplish a well-defined objective

IRI PRACTICE AREAS

User experience practice will ensure relentless attention to user perspectives and needs through requirements gathering, user-centric (co)-design, continuous feedback, and other means.

Resource co-operations practice is focused on creating new modes of cooperation, collaboration, co-scheduling, and joint planning across facilities and DOE programs.

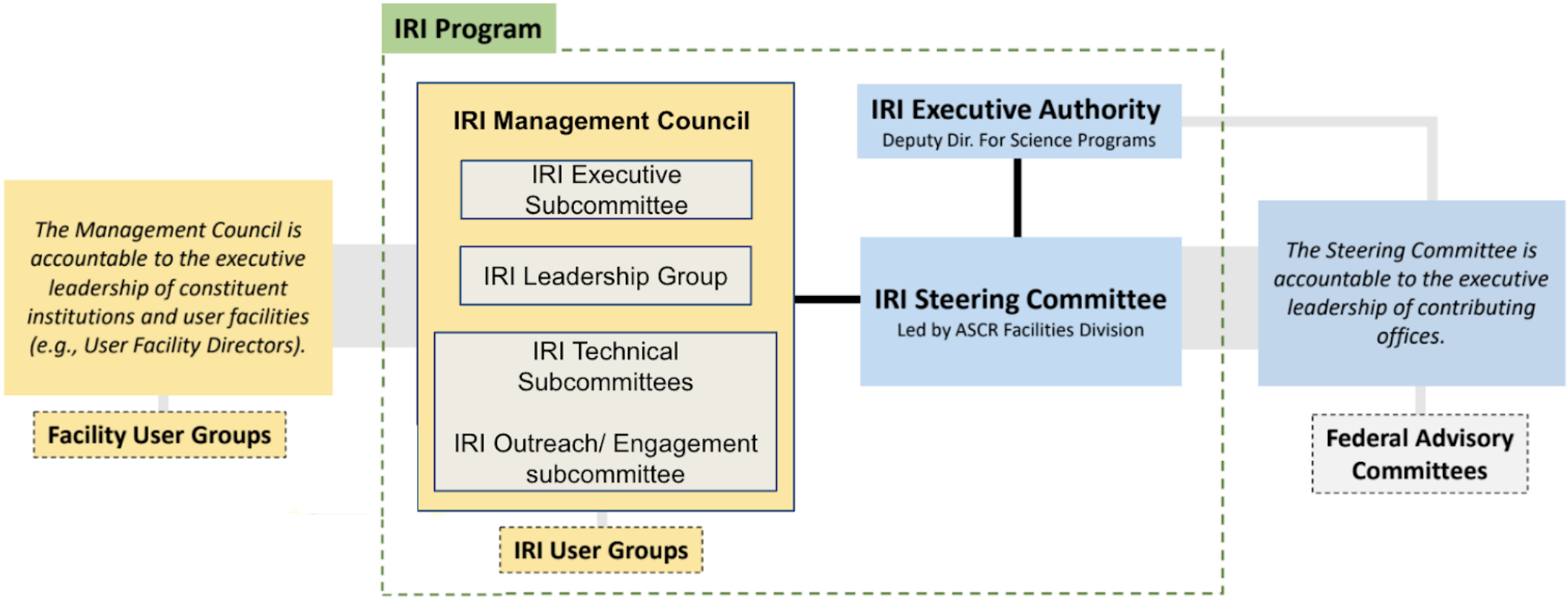
Cybersecurity and federated access practice is focused on creating novel solutions that enable seamless scientific collaboration within a secure and trusted IRI ecosystem.

Workflows, interfaces, and automation practice is focused on creating novel solutions that facilitate the dynamic assembly of components across facilities into end-to-end IRI pipelines.

Scientific data life cycle practice is focused on ensuring that users can manage their data and metadata across facilities from inception to curation, archiving, dissemination, and publication.

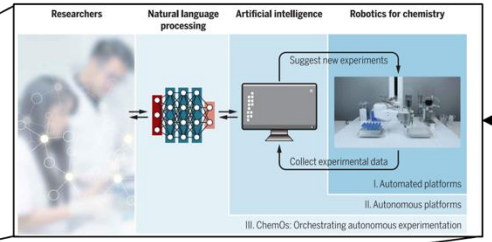
Portable/scalable solutions practice is focused on ensuring that transitions can be made across heterogeneous facilities (portability) and from smaller to larger resources (scalability).

IRI Program Governance

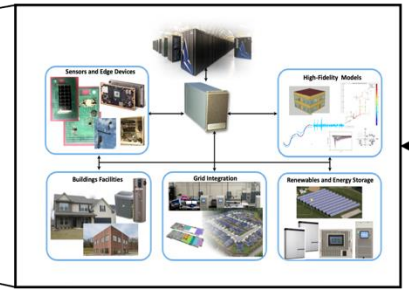


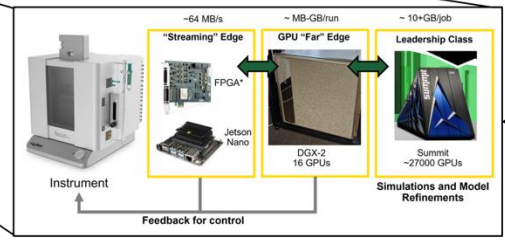
Interconnected Smart Labs of the Future (2030+)

Materials Lab



Electric Grid Lab





Microscopy Lab

Interconnected Smart Labs

Interoperable Ecosystem is Required
Seamless Edge-to-HPC

INTERSECT
INTERCONNECTED SCIENCE ECOSYSTEM

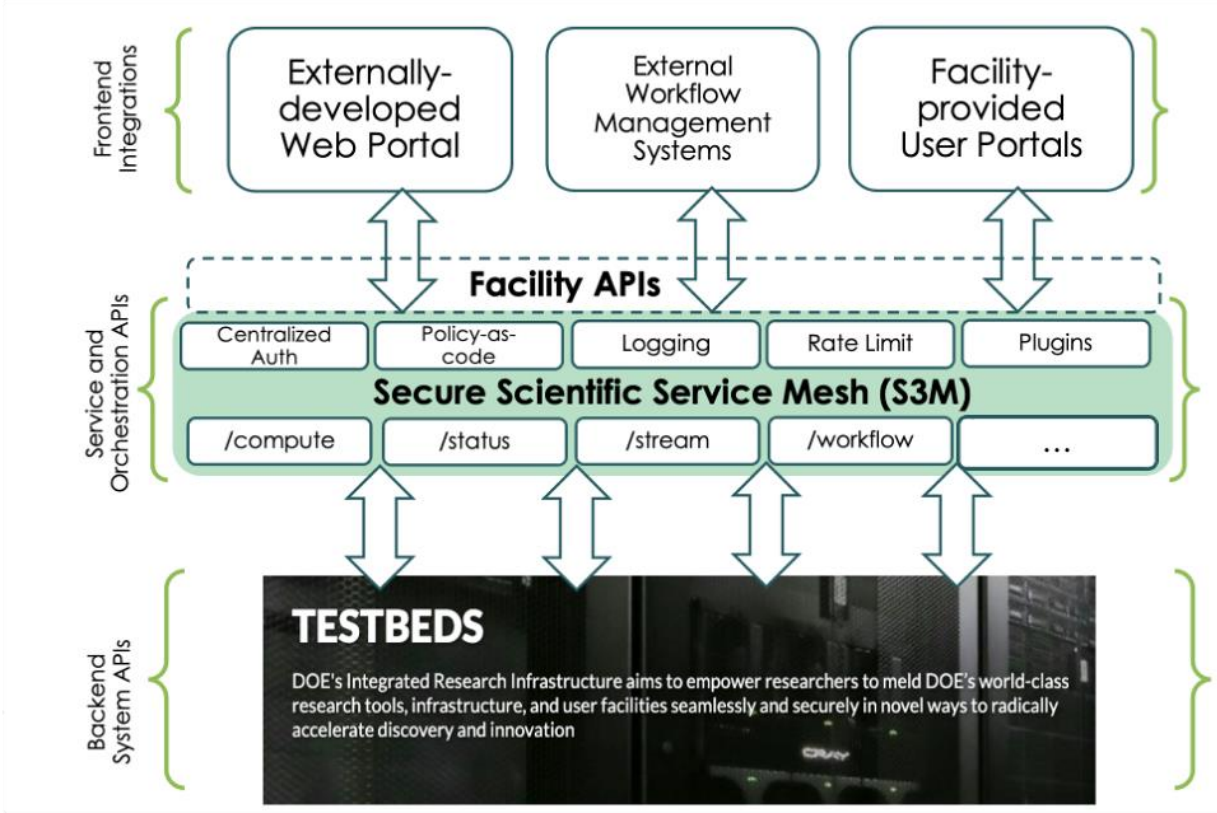
Secure Scientific Service Mesh (S3M)

S3M LAYER BUILT UPON A K8S-BASED OPENSHIFT SYSTEM AND ISTIO SERVICE MESH

- Sits between third-party systems and protected resources
- Decoupled service layer from HPC systems
- Enables secure, monitor, customizable, and scalable service interfaces in support of autonomous science

SECURITY-FIRST MINDSET

- Provides a central service that is capable of enforcing policy, logging, authenticating, authorizing, and securing all income API requests to a range of target systems



IRI ACE Testbed

Explore new **policies** and **technologies** to enable IRI, INTERSECT, and OLCF-6

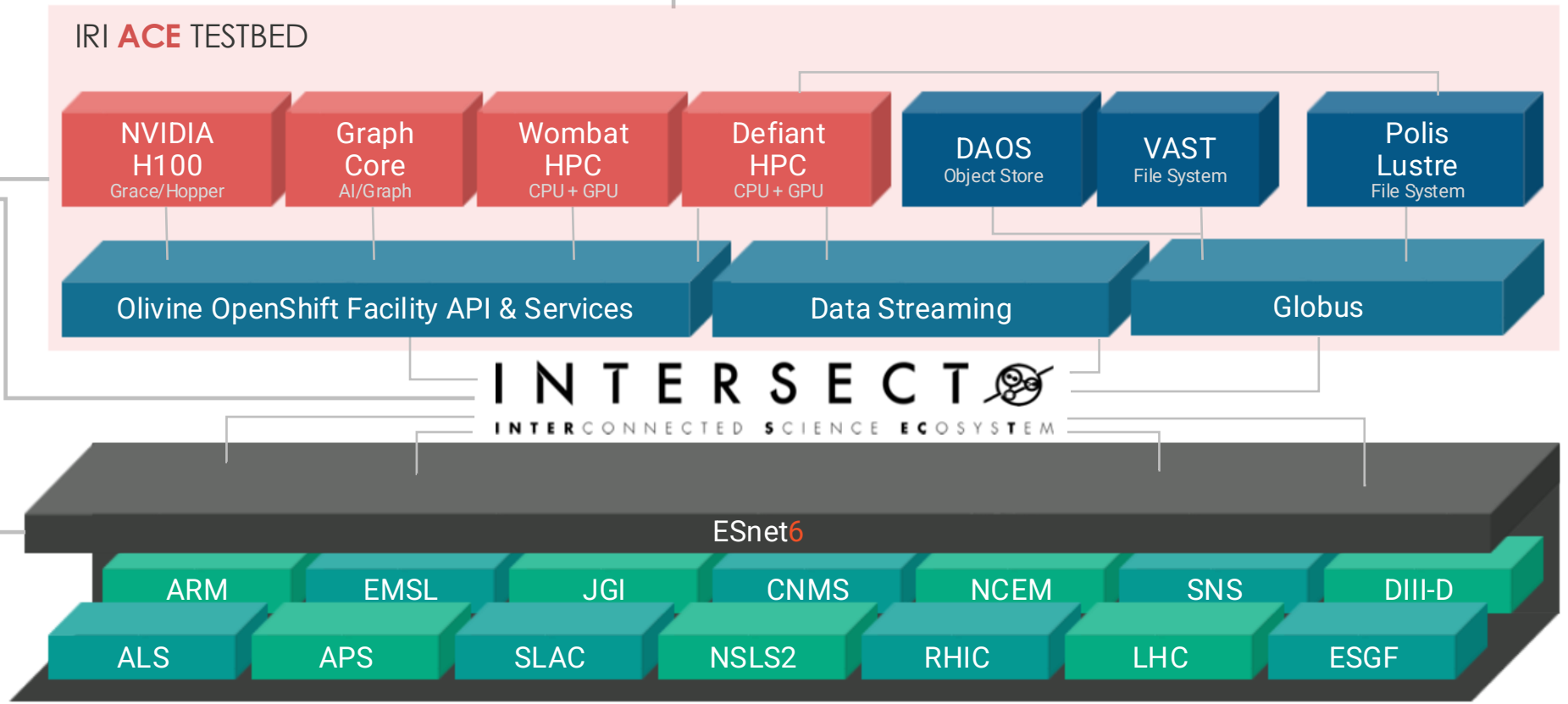
Enabling **INTERSECT** use cases and communication via a common message layer

A **unique sandbox environment** to design, develop, and evaluate secure workflows connecting DOE science facilities to OLCF

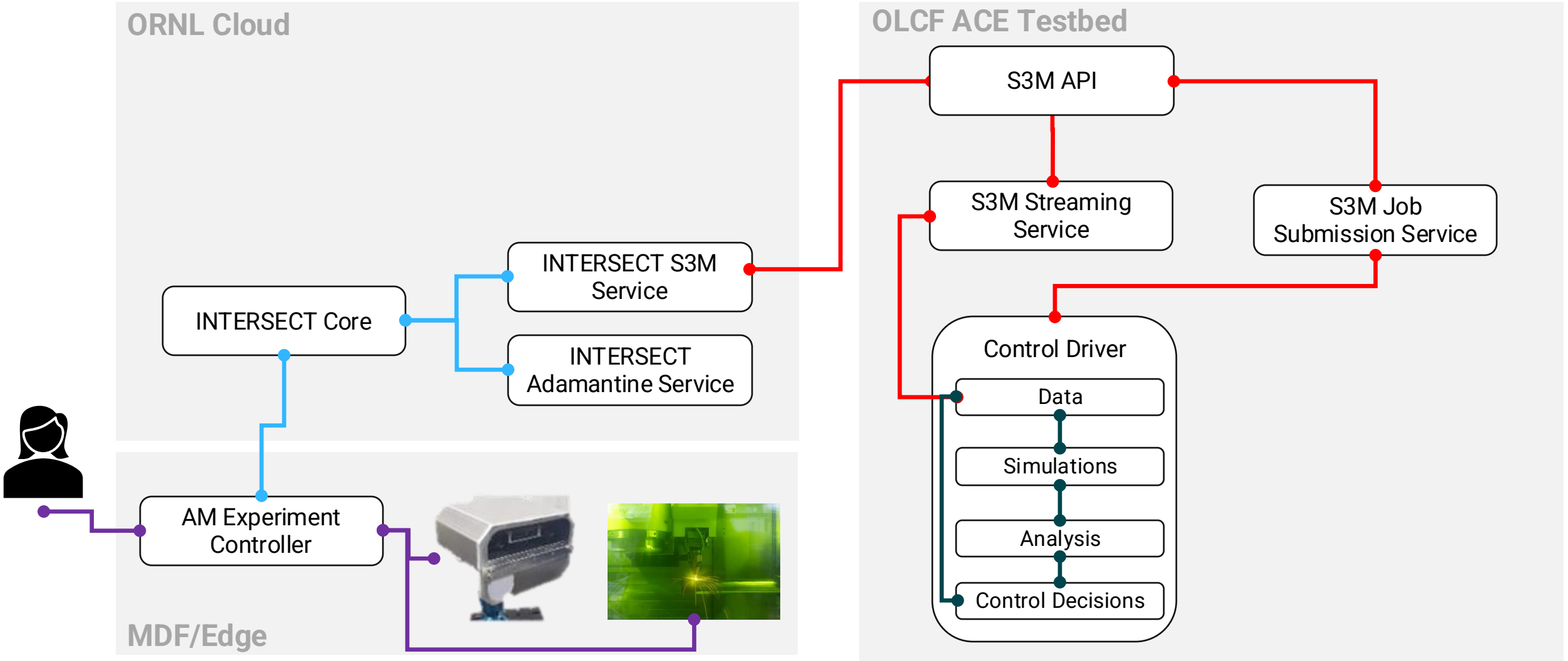
Open Development

non-production resources

- Diverse **Computing** and **Storage** systems
- Interoperable **APIs** and **Services**



Use Case: Autonomous Additive Manufacturing Workflow



WfBench: A Comprehensive Workflow Benchmarks Suite

Bridge the gap between traditional HPC AND AI-INTEGRATED WORKFLOWS

Evaluation of HPC system capabilities for running workflow applications

Support for diverse computing environments (HPC, CLOUD, EDGE, QUANTUM)

Multi-facility workflow assessment and DATA MANAGEMENT

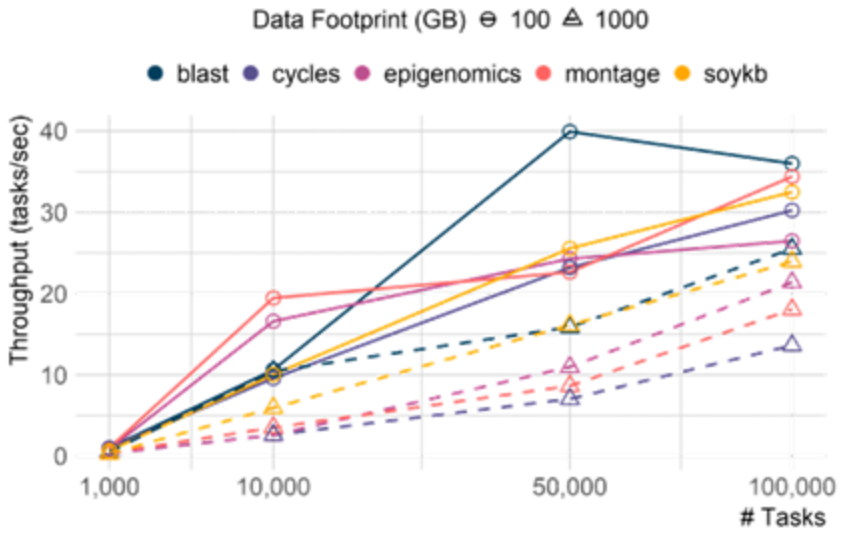
ENERGY EFFICIENCY measurement and optimization

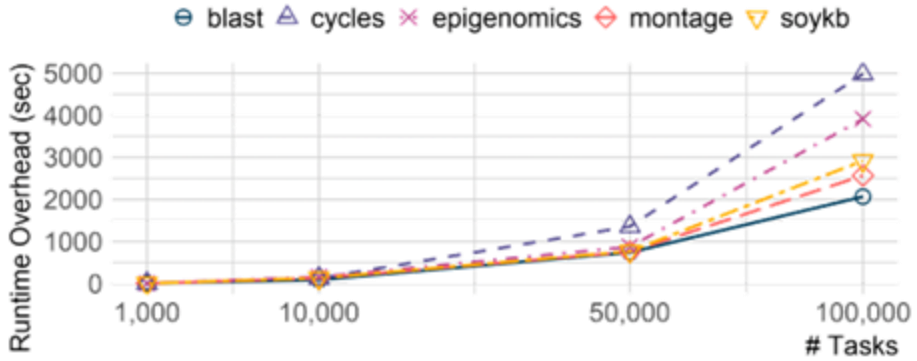
TIME-SENSITIVE workflow evaluation capabilities

All workflows perform the **same amount of work**

↑ data footprint ↓ throughput

↑ #tasks ↑ throughput

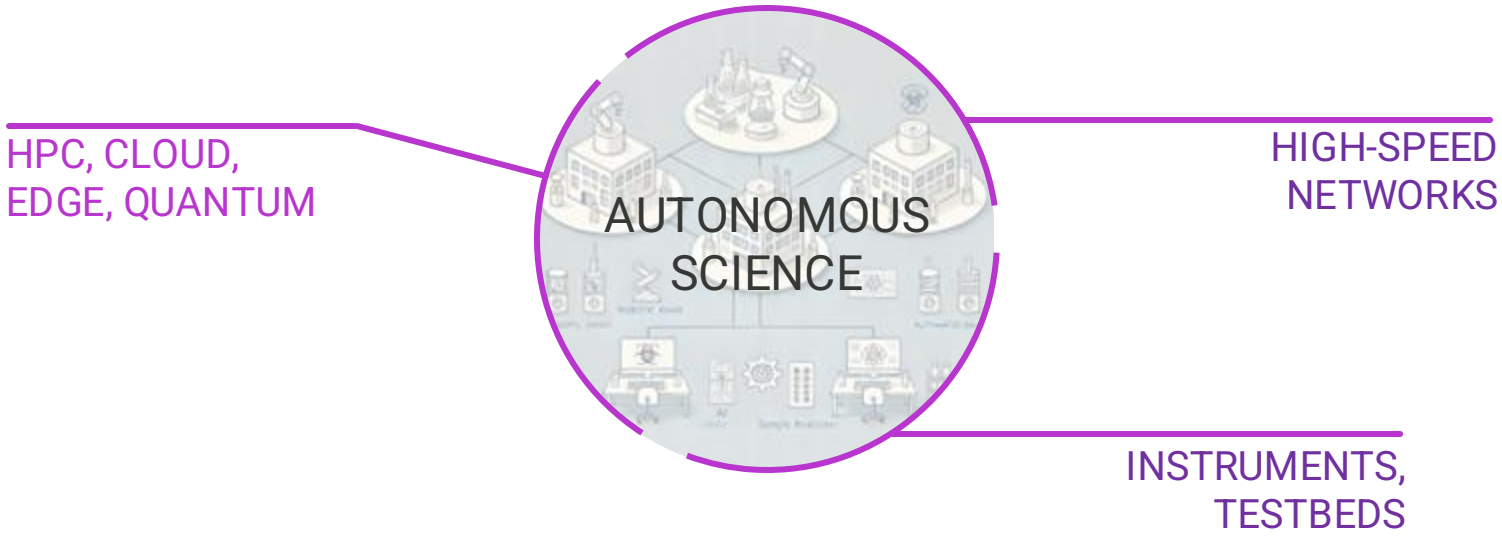




WfBench: Automated Generation of Scientific Workflow Benchmarks

T. Coleman, et al., PMBS 2022

https://doi.org/10.1109/PMBS56514.2022.00014


HPC, CLOUD,
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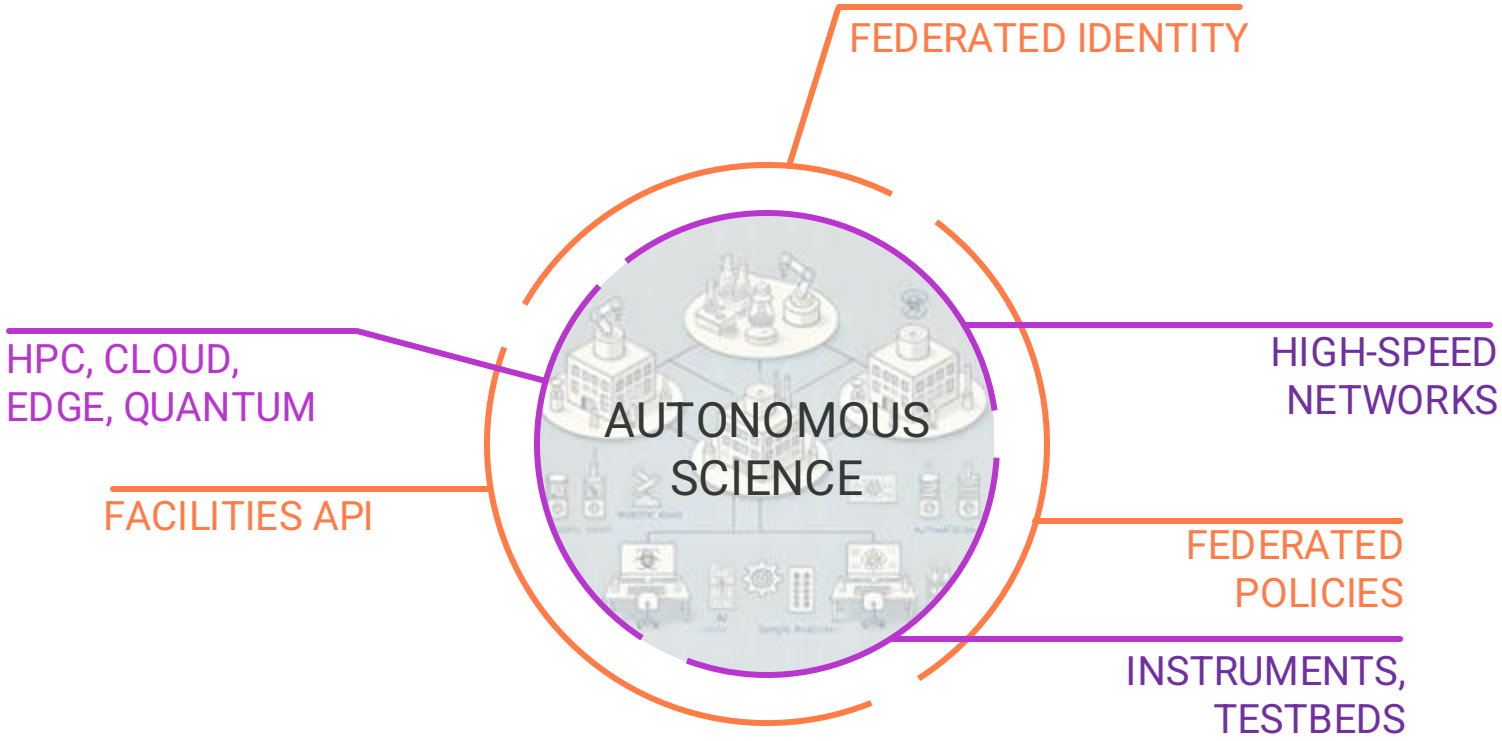
TESTBEDS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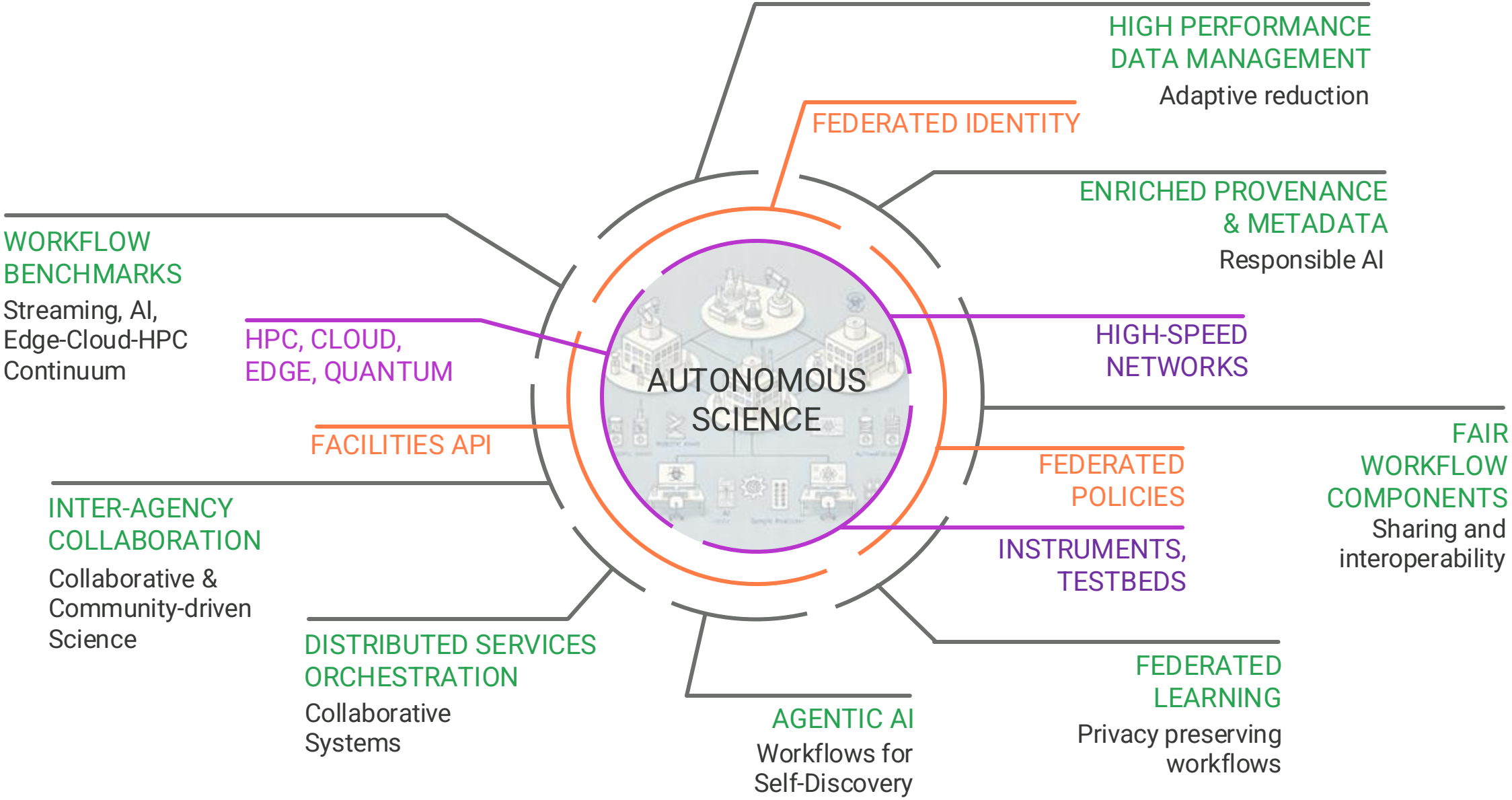
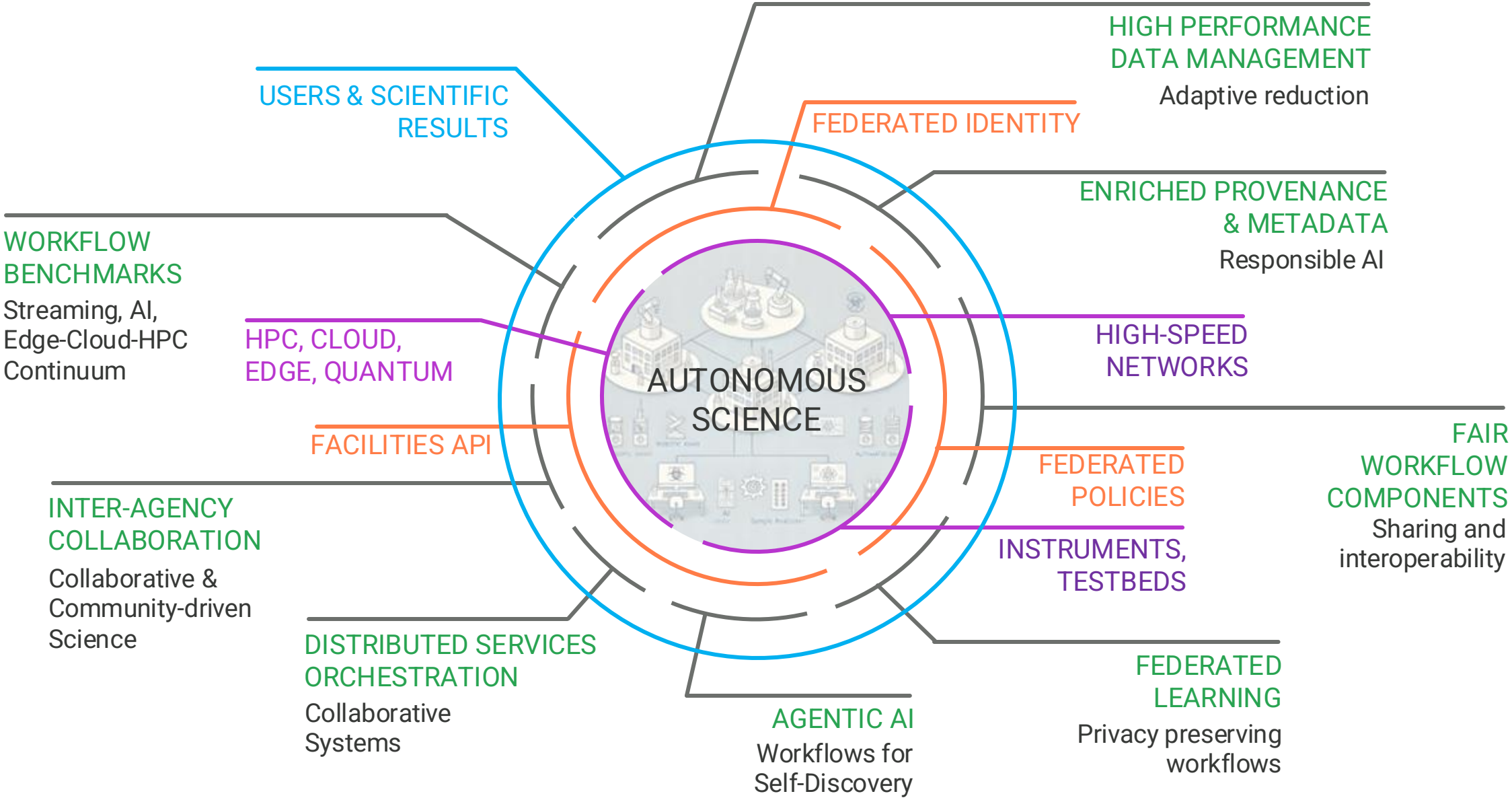

HIGH PERFORMANCE DATA MANAGEMENT
Adaptive reduction
FEDERATED IDENTITY
ENRICHED PROVENANCE & METADATA
Responsible AI
WORKFLOW BENCHMARKS
Streaming, AI, Edge-Cloud-HPC Continuum
HPC, CLOUD, EDGE, QUANTUM
HIGH-SPEED NETWORKS
AUTONOMOUS SCIENCE
FACILITIES API
FAIR WORKFLOW COMPONENTS
Sharing and interoperability
FEDERATED POLICIES
INTER-AGENCY COLLABORATION
Collaborative & Community-driven Science
INSTRUMENTS, TESTBEDS
DISTRIBUTED SERVICES ORCHESTRATION
Collaborative Systems
FEDERATED LEARNING
Privacy preserving workflows
AGENTIC AI
Workflows for Self-Discovery


USERS & SCIENTIFIC RESULTS
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Thank You!

Questions?

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