

Interconnected Science Ecosystem (INTERSECT) Initiative

Ben Mintz, Director of INTERSECT

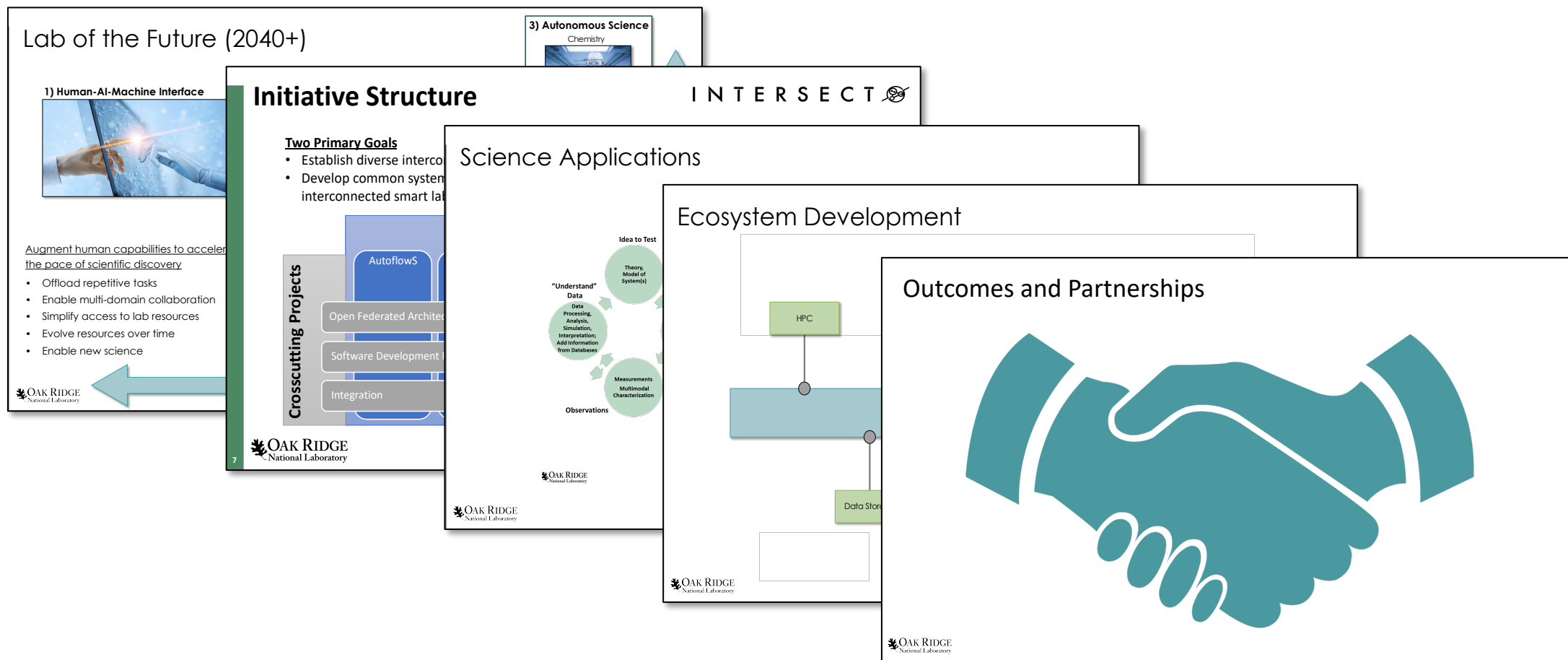
Elke Arenholz, Director of INTERSECT

April 25, 2022

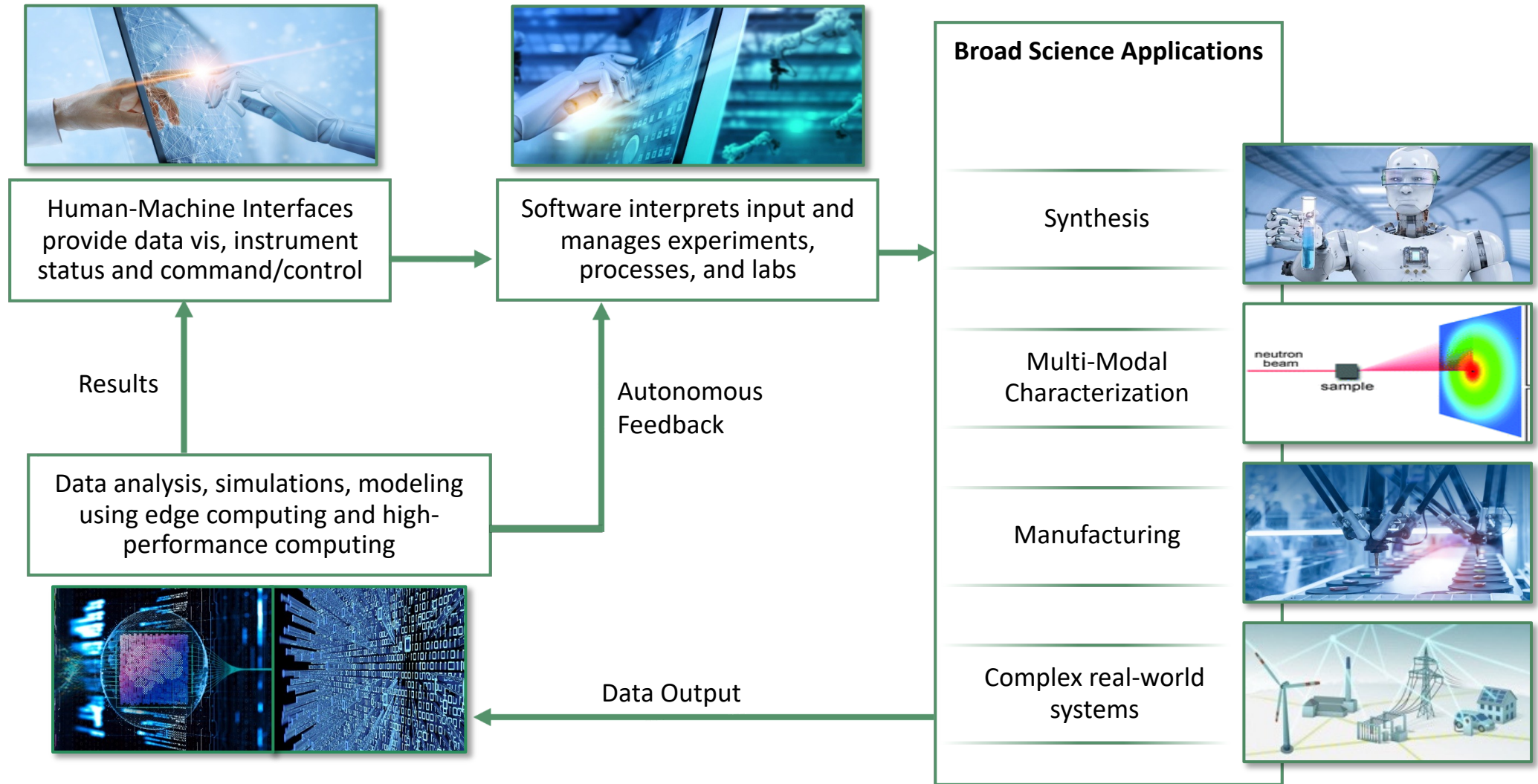
ORNL is managed by UT-Battelle LLC
for the US Department of Energy

Overview

Primary Goal - Develop and implement a scalable One-ORNL system-of-systems (SoS) ecosystem to enable smart, “self-driving” experiments and processes that accelerate the pace of scientific discovery

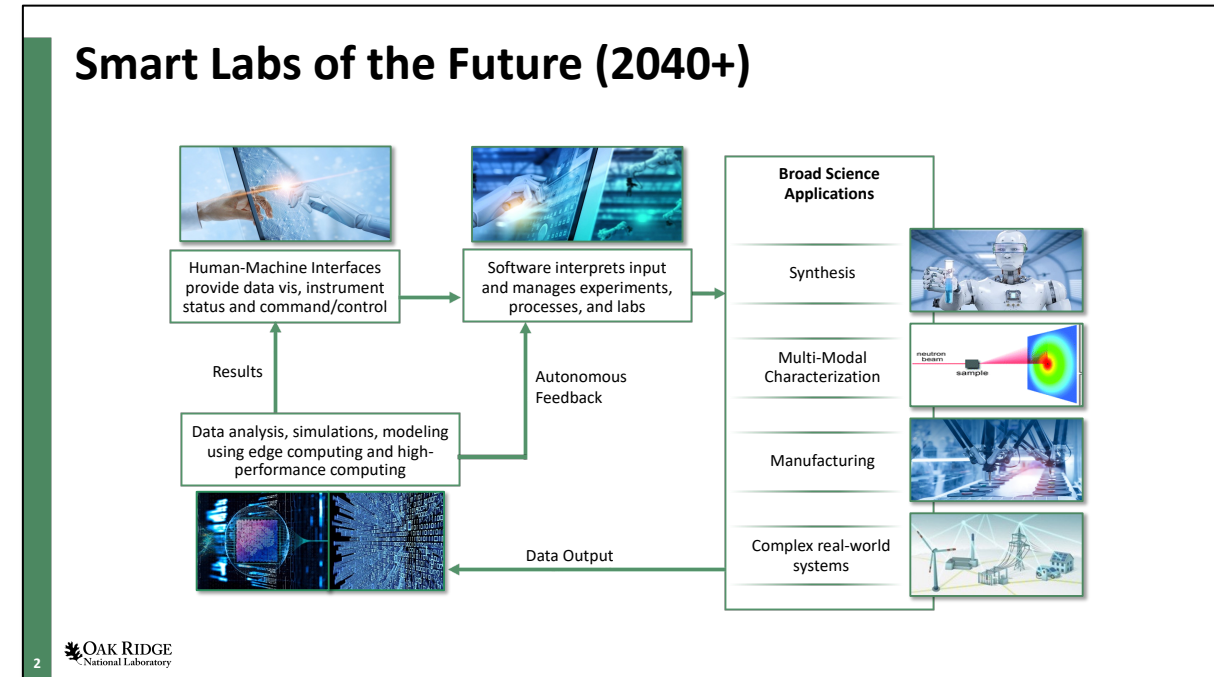


Smart Labs of the Future (2040+)



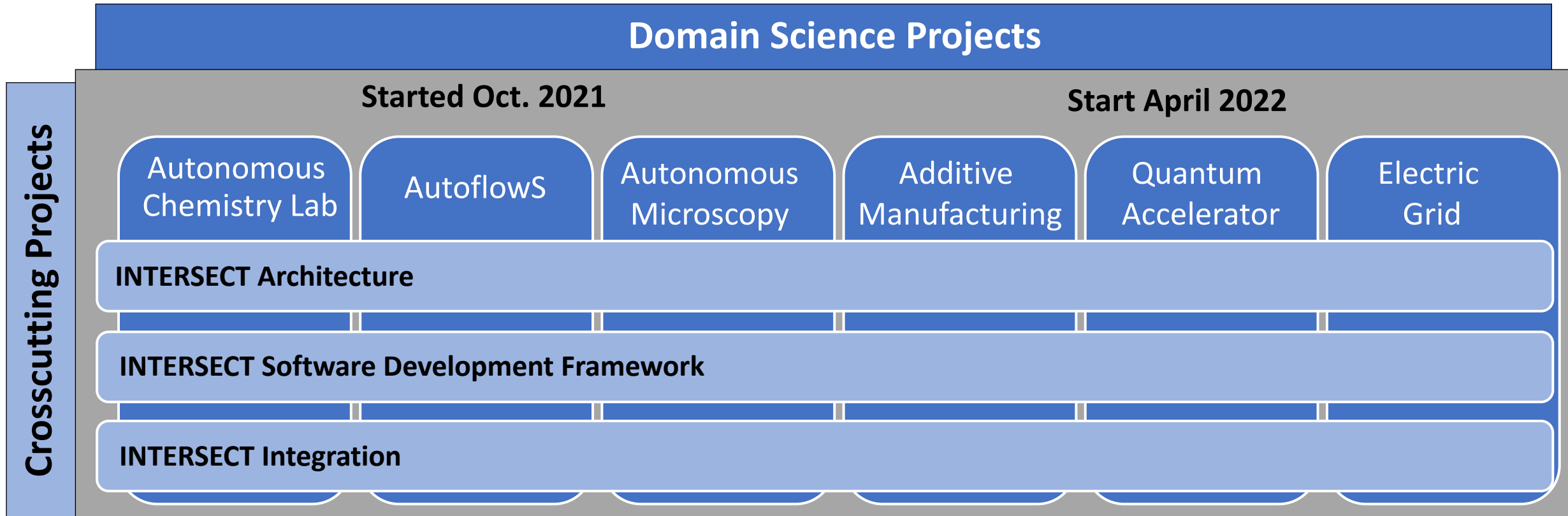
Challenge for Interconnected Labs

- Lack of coordination across smart lab projects
 - Common solutions are reinvented
 - Data and messaging infrastructure
 - Software functionality
 - Hardware solutions and integration efforts
 - Interoperability becomes complex, or impossible as the number of solutions increase
 - Solutions do not scale beyond a single domain and/or application
 - Cyber security is an afterthought or ignored



Common ecosystem is required for interconnected smart labs of the future

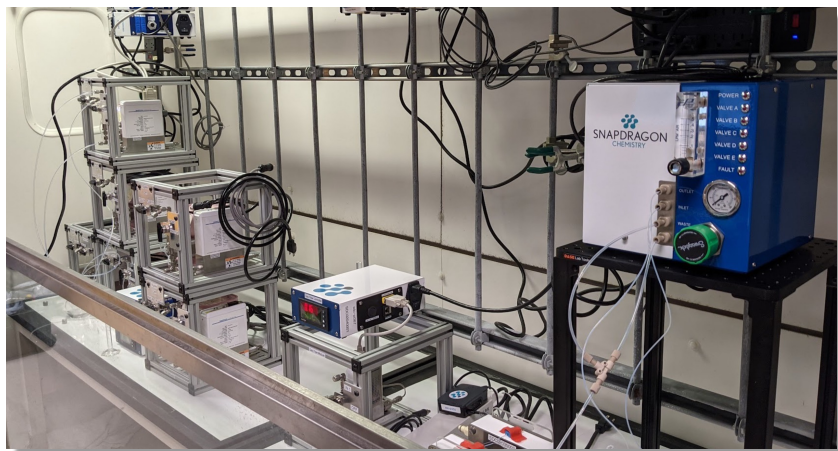
INTERSECT Initiative Programmatic Structure



Domain Science Projects (Started Oct. 2022)

Autonomous Continuous Flow Reactor Synthesis (AutoFlowS)

R. Advincula, CNMS
B. Sumpter, CNMS

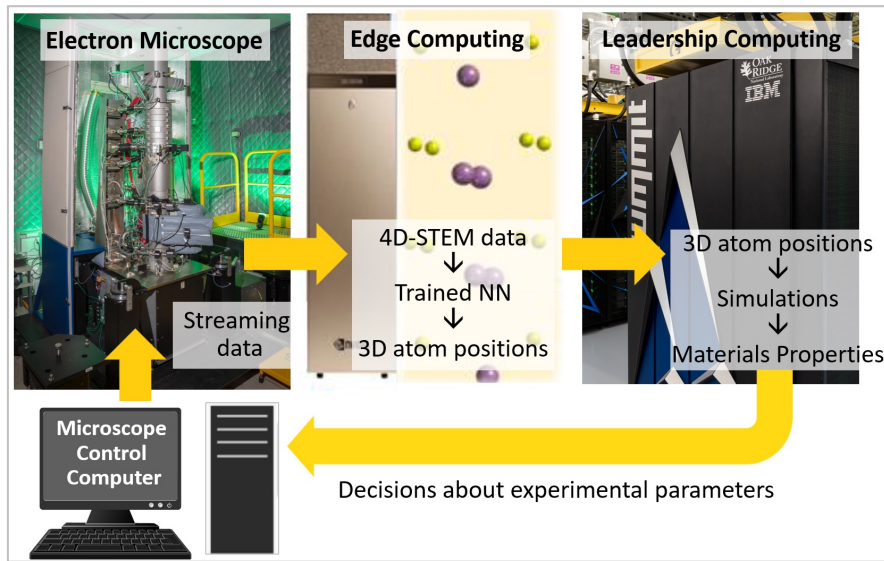


Develop automated, ultimately autonomous continuous flow chemistry system combining in-situ/operando characterization capabilities (e.g. UV/Vis, IR, NMR) with AI-enabled analysis/feedback

Autonomous Microscopy

M. Ziatdinov, CNMS
S. Kalinin, CNMS

Establish data streaming, on-the-fly data analysis and simulation for AI-enabled feedback for microscopes at CNMS



Autonomous Chemistry Lab, ACL

S. Dai, CSD



B. Burger et al., Nature 583, 237 (2020)

Establish an autonomous robotic chemistry lab that operates 24/7

Domain Science Projects (Starting April 2022)

Enabling adaptively controlled additive manufacturing through automation

S. DeWitt, CSED

Ion Trap Quantum Computing Resource:
Optimization and Access

C. Seck, CSED

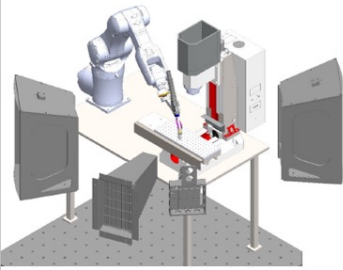
Autonomous additive manufacturing (AM) enabled by combining AM build system, in-situ characterization, and on-the-fly simulations.

S. Debnath, ESTD

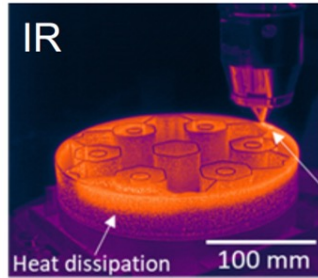
Establish scalable platform for emulation of large scale energy system and power grids

Develop autonomous optimization of ORNL's trapped ion quantum resource and provide user access through INTERSECT

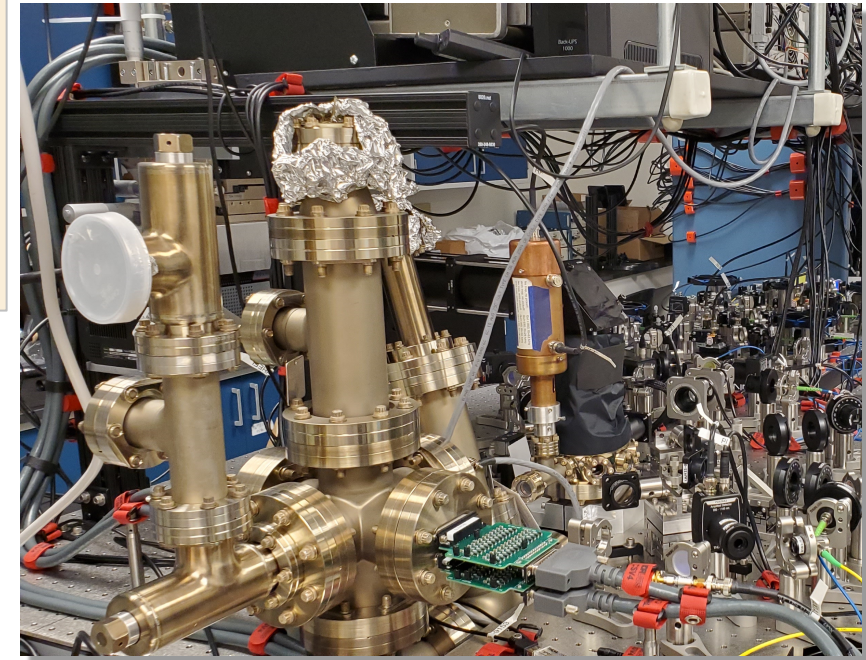
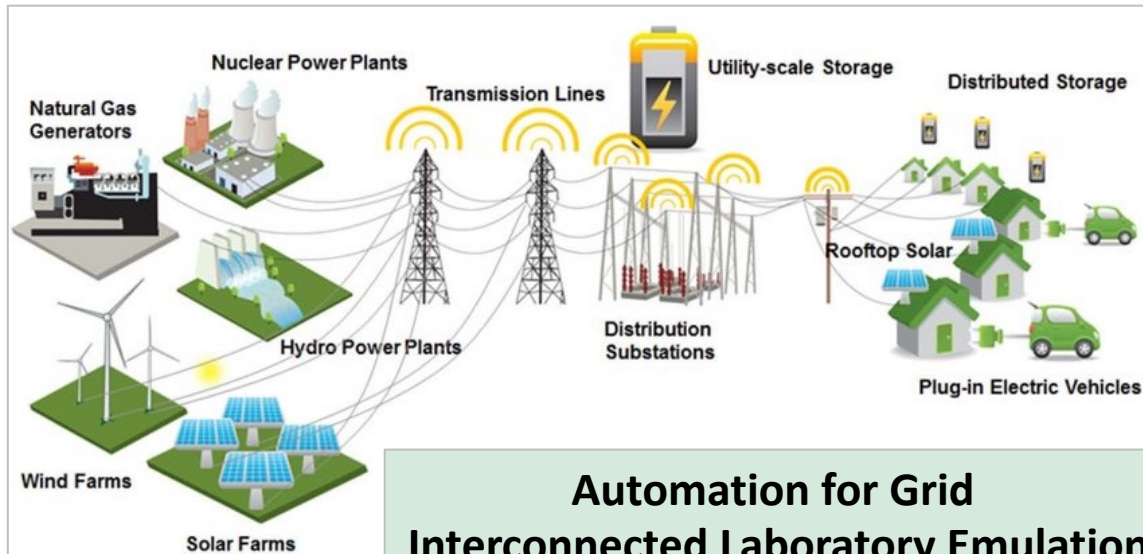
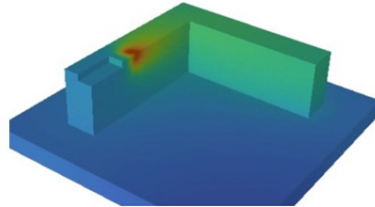
Additive Manufacturing



In-situ Characterization

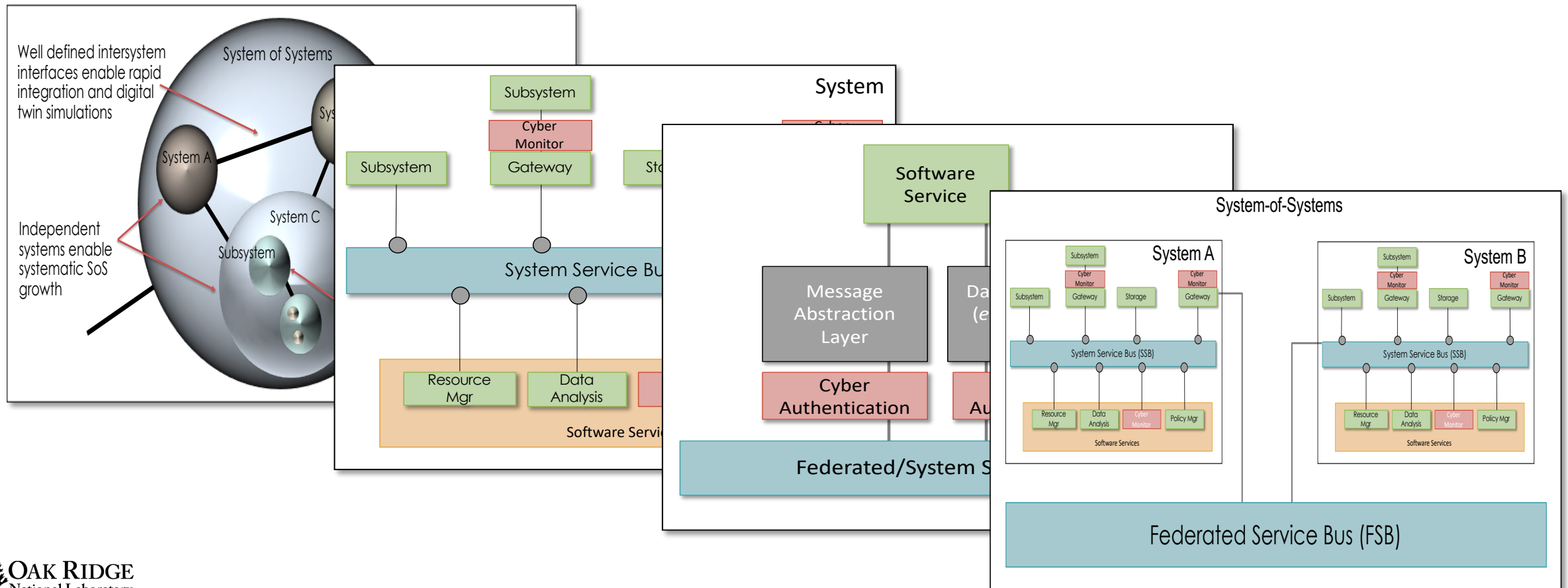


Thermomechanical Simulations

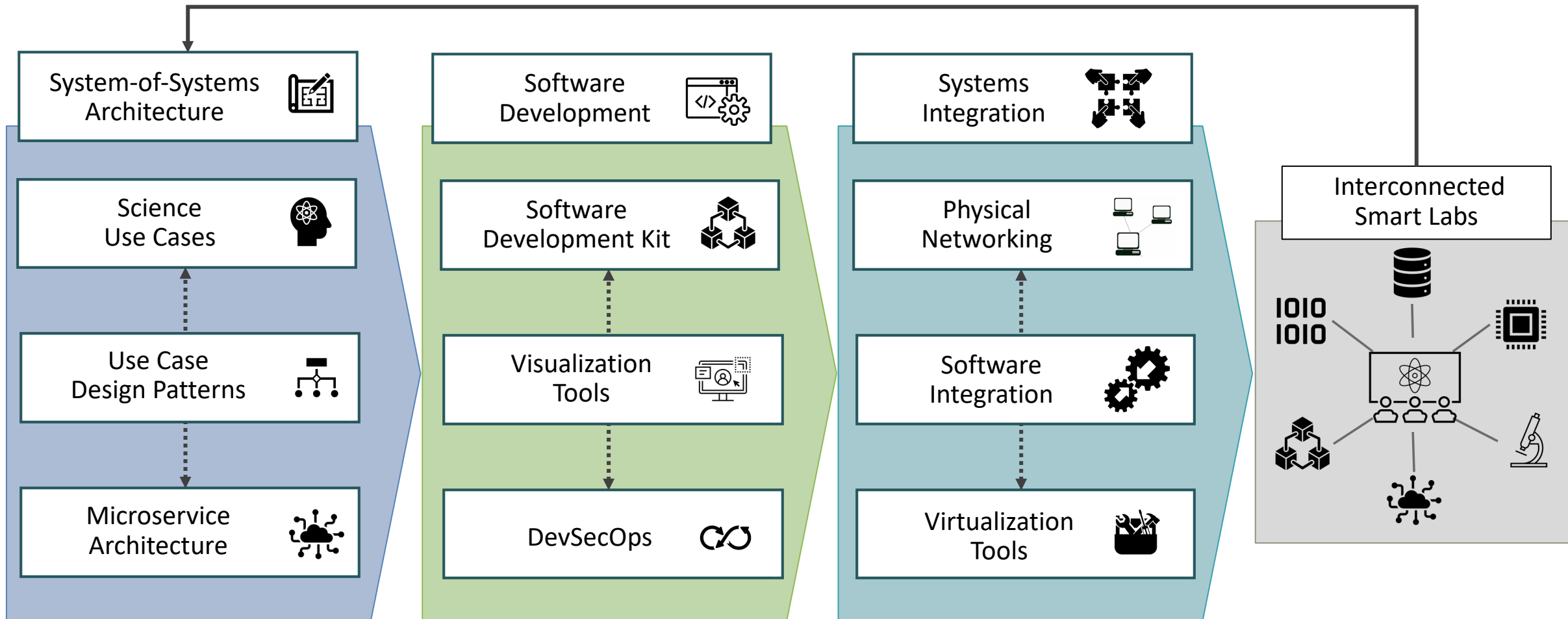


SoS and Microservice Architecture

- System-of-Systems (SoS) is a node agnostic solution in which component systems combine to provide more functionality than the individual pieces
- Define architecture elements for a system
- Cyber security can monitor internal/external system traffic

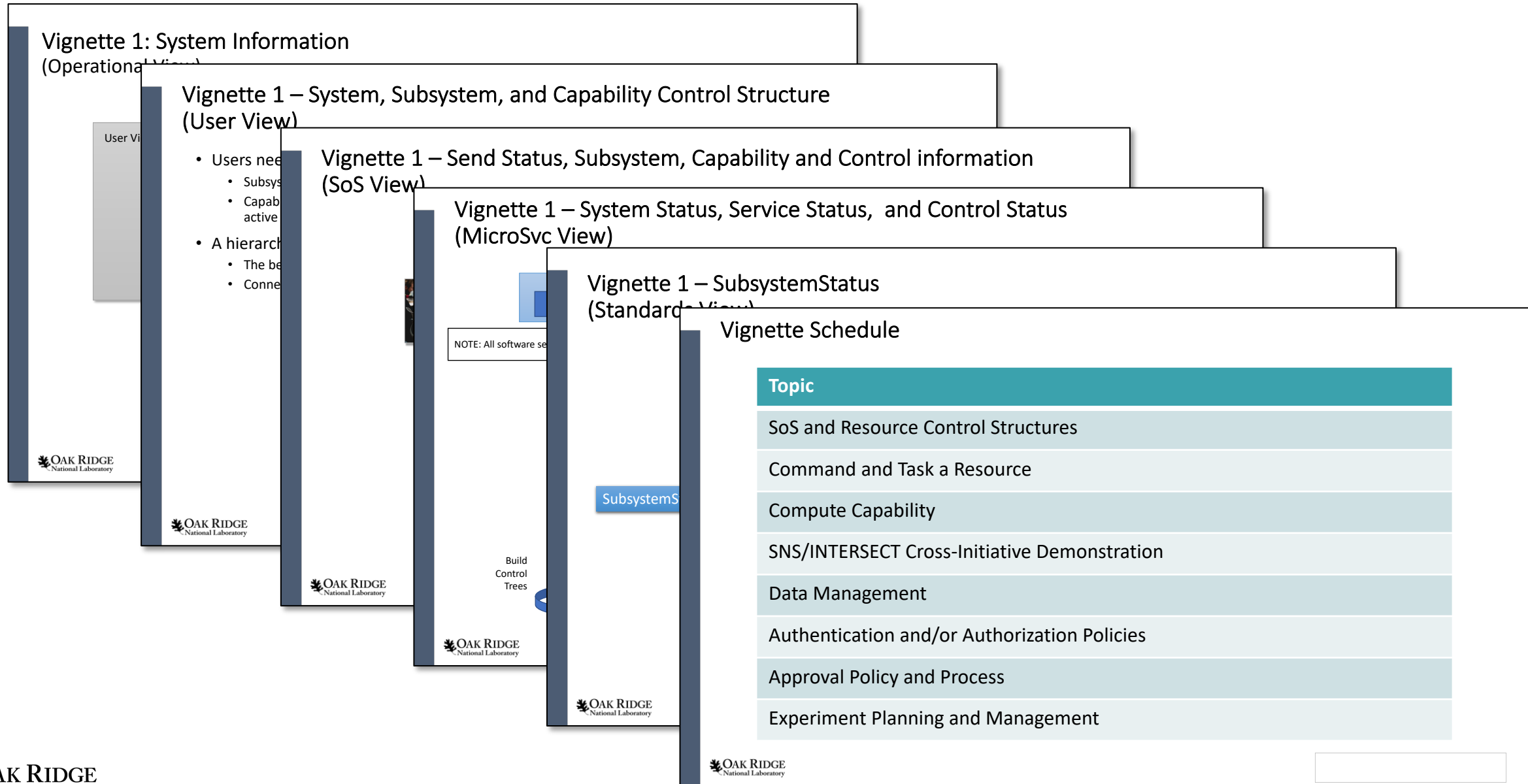


INTERSECT Crosscutting Projects



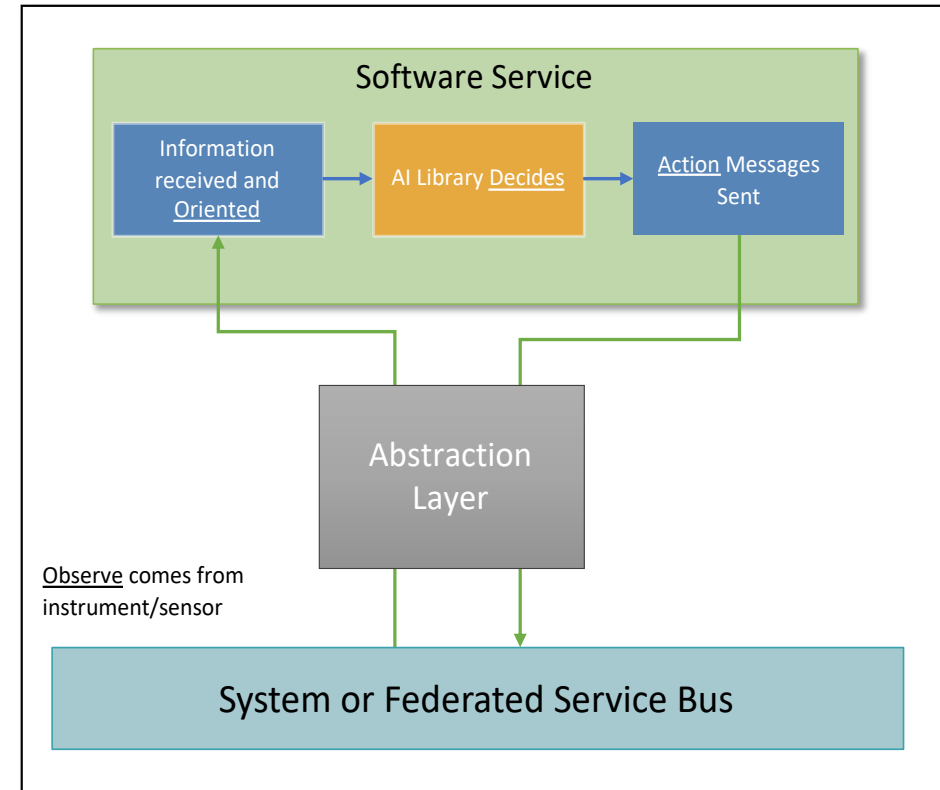
Crosscutting Projects Build and Integrate the Common Solutions Required for an Integrated Multi-Domain Science Ecosystem

Develop Architecture Viewpoints



AI/INTERSECT Integration

- AI Initiative is developing AI libraries for ORNL
 - Surrogates and design (*e.g.*, ML for multiscale materials and AI-based materials design/co-design)
 - Imaging (*e.g.*, physics-informed ML and Bayesian methods)
 - Engineering and Science (*e.g.*, digital twins, anomaly detection, and edge control systems)
 - Assurance (*e.g.*, Verification/Validation and Causal Analysis)
- INTERSECT provides a technology transition pathway for AI/ML algorithms
 - AI/ML libraries are wrapped within an INTERSECT software service
- AI/ML adds the "smart" into ORNL Smart Labs
 - Experiment Planning/Steering
 - System and/or SoS Contingency Management
 - AI/ML Control Systems (*e.g.*, Instrument and sensor controls)
 - Cyber Monitoring
 - Data Analysis



Potential Partnerships

- INTERSECT initiative started October/November 2021
 - Draft SoS architecture is complete
 - Demonstrated command and control plan messaging
 - Building initial orchestration microservices
 - Autoflows reactor installed at ORNL and initial test reactions complete
 - Building electron microscopy automation and integrating AI solutions



Questions?

