INTERSECT MULTIBUS: Interconnected Science Ecosystem for Multi-Facility Autonomous Experiments

Laboratory Directed Research & Development

LDRD.ORNL.GOV

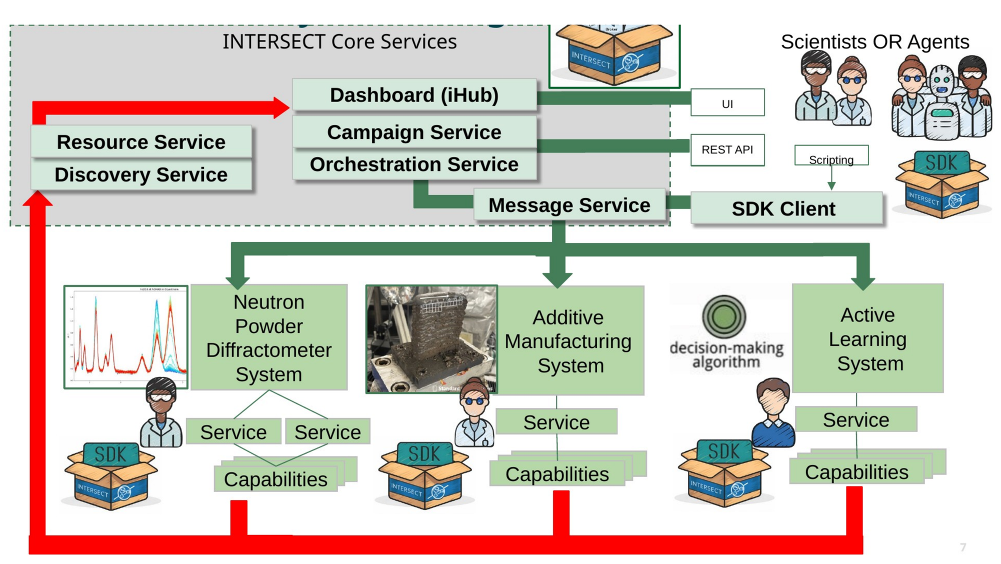
PROGRAM: Director's R&D (DRD)
INITIATIVE: Interconnected Science Ecosystem (INTERSECT)
PI: Marshall McDonnell (CSMD)
CO-I(S): L. Drane, G. Cage, P. Bryant, R. Archibald, M. Brim, S. Hitefield, A. Ghosh, S. DeWitt, C. Fancher, A. Malviya-Thakur
CONTRIBUTOR(S): ORNL — A. Shrivastava, S. Venkatakrishnan, J. Ramirez Osorio, P. Laiu, R. Gregory, K. Gofron, B. Vacaliuc, Z. Thurman, G. Wiggins, J. McGaha, A. Ayres, R. Smith, G. Watson, J. Liu, M. Doucet, M. Backman, C. Bridges, M. Tucker, E. Van Auken, L. Daemen, T. Proffen, M. Kirkham, D. Rosendo, T. Skluzacek, R. Prout, B. Mintz, R. Moore | CHESS/Cornell — K. Shanks, A. Das, W. Sun, K. Nygren, S. Sarker | NIST — A. McDannald, A.G. Kusne, W. Ratcliff, T. Martin | NSDF (UTK / U. Utah) — M. Taufer, J. Marquez, K.H. Ng, V. Pascucci, G. Scorzelli, A. Gooch

1. WHAT IS INTERSECT?

Autonomous experiments need instruments, simulations, data services, and decision-making algorithms to talk to each other — usually across facility, network and security boundaries. We need an ecosystem to swap instruments, compute, and decision-making to fit the science use case.

INTERSECT (Interconnected Science Ecosystem) is a system-of-systems design to bring any instrument, simulation, analysis tool, or decision-making algorithm into a shared ecosystem as a Service that exposes typed Capabilities.

- Autonomy is a spectrum — deterministic logic, simulation feedback, machine learning surrogates, agentic AI. Mix and match: swap the instrument, swap the analysis, swap the decision-maker.
- 12 use cases, 6 of 8 ORNL directorates, multiple institutions; deployed at ORNL, the National Science Data Fabric, NERSC and AWS.



INTERSECT ecosystem design: core services provide discovery, messaging, resource tracking, campaigns and orchestration; scientists — or AI agents — drive the ecosystem through the SDK client, a REST API, or the iHub dashboard.

2. HOW TO CONNECT TO INTERSECT: SDK

The INTERSECT Software Development Kit (SDK) is how an instrument, simulation, or data service connects to the ecosystem. Write a Python class, decorate its methods with @intersect_message, add event publishers, and the SDK generates and broadcasts a typed schema to the ecosystem. The SDK supports a pluggable Message Abstraction Layer (currently MQTT and AMQP). Services appear in the iHub dashboard and can be driven as campaigns through the Campaign Orchestrator.

```
class HelloServiceCapabilityImplementation(IntersectBaseCapabilityImplementation):

    intersect_sdk_capability_name = 'HelloExample'

    @intersect_status()
    def status(self) -> str:
        """Basic status function which returns a hard-coded string."""
        return 'Up'

    @intersect_message()
    def say_hello_to_name(self, name: str) -> str:
        """Takes in a string parameter and says 'Hello' to the parameter!"""
        return f'Hello, {name}!'
```

A complete INTERSECT capability — two decorated methods are all that is needed to put a new instrument, code or algorithm into the ecosystem.

MULTIBUS: security for real campaigns

Authentication and authorization was the critical-path bottleneck for multi-user, multi-facility campaigns. MULTIBUS built the missing pieces:

- INTERSECT Keycloak at ORNL, federated to ORNL SSO and to iHub for single sign-on; validated against both OIDC and SAML identity providers.
- Registry Service: authenticated users reserve a service namespace with an API key, so system credentials stay server-side, not in service code.
- Hybrid RSA + AES message encryption in the SDK — encrypts MB-scale payloads with negligible size overhead, agnostic to message type or schema.
- Campaign Orchestrator built on Petri nets for cyclic, event-driven campaigns; broker HTTP proxy to bridge INTERSECT deployments across networks.
- SDK releases 0.1.0 → 0.9.0, a shared Common library, and Helm charts for every core service. github.com/INTERSECT-SDK

3. AUTONOMOUS ADDITIVE MANUFACTURING

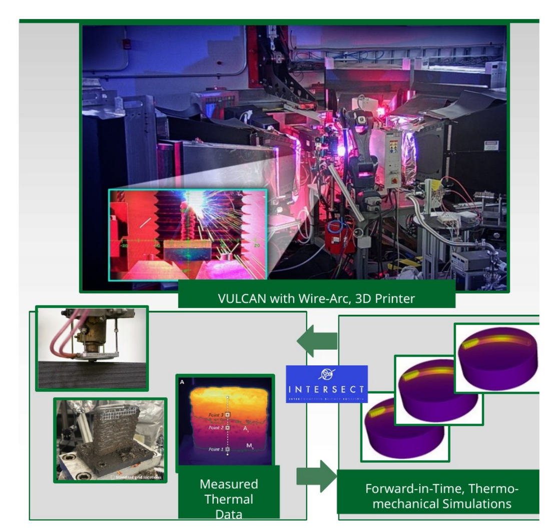
Goal: Metal parts that are "born qualified" — printed and ready to use without extensive post-build qualification. Part quality is exquisitely sensitive to process parameters, and the design space is far too large to search by hand.

- Nov. 2024 — Spallation Neutron Source (SNS) Engineering Materials Diffractometer (VULCAN):

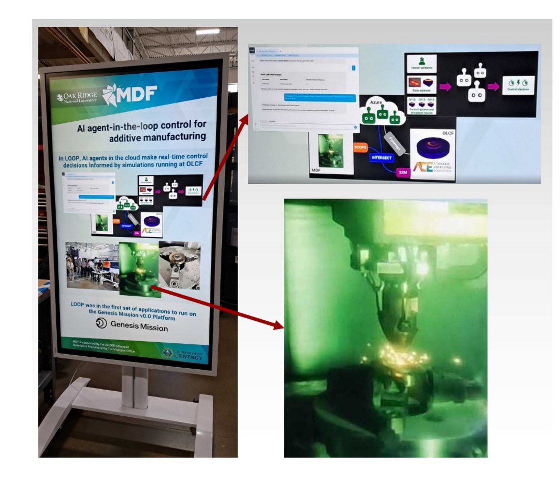
  A wire-arc directed energy deposition printer ran on the VULCAN beamline, one layer every ~1–2 min. Infrared thermal data was assimilated into forward-in-time thermomechanical simulations using adamantine: github.com/adamantine-sim/adamantine. Model-predictive control adapted power, velocity, and wire feed. Neutron strain data was collected concurrently.

- Sep. 2025 — Manufacturing Demonstration Facility (MDF) and Oak Ridge Leadership Computing Facility (OLCF):

  Live print at the MDF steered by simulations on OLCF testbed machines, with agentic AI constructing and launching the workflow, injecting decisions during the print, and auditing data provenance. Also shown at SC25 and among the first applications on the Genesis Mission platform (Rosendo et al., SC25-W, doi:10.1145/3731599.3767592).



VULCAN with the wire-arc printer; thermal data feeds the simulations that steer the next layer.



The Sep. 2025 live print at the MDF, steered by OLCF simulations with AI agents in the loop.

4. AUTONOMOUS NEUTRON SCATTERING

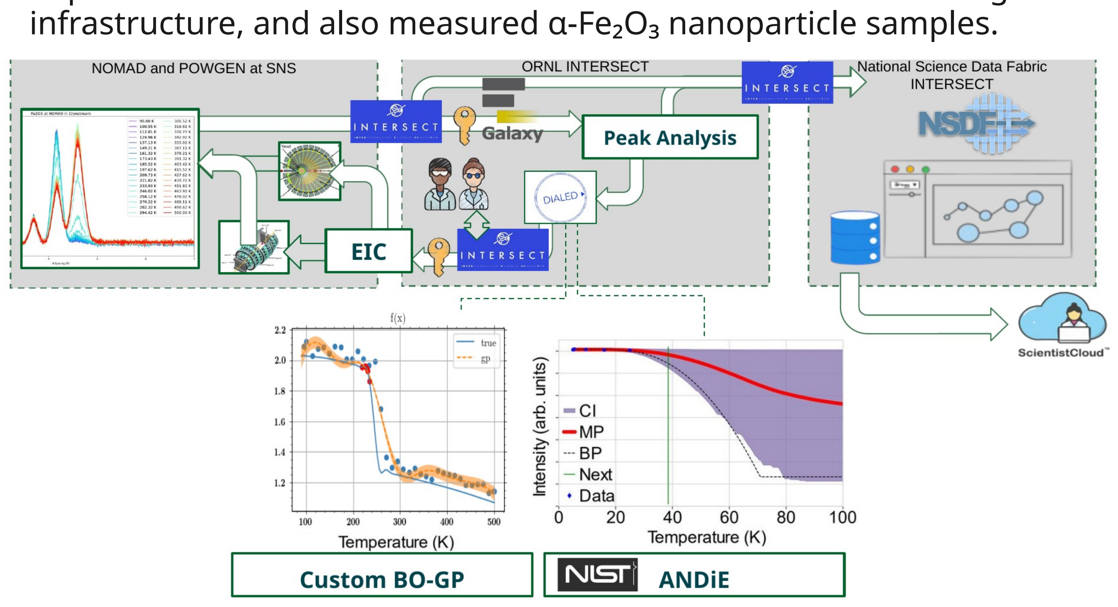
Goal: Autonomously explore phase transitions via neutron scattering while swapping instruments and decision-making algorithms.

- May 2025 — SNS Nanoscale-Ordered Materials Diffractometer (NOMAD):

  Autonomous neutron diffraction on NOMAD mapped the α-Fe_2O_3 (hematite) Morin transition near 260 K, steered by INTERSECT. A custom Bayesian-optimization Gaussian process and the NIST ANDiE physics-informed algorithm were both served through DIAL, the Distributed INTERSECT Active Learning service.

- Sep. 2025 — SNS POWGEN Powder Diffractometer:

  Repeated the autonomous neutron diffraction on POWGEN using the same infrastructure, and also measured α-Fe_2O_3 nanoparticle samples.



The same ecosystem, reused across two beamlines: NOMAD in May 2025 and POWGEN in Sep. 2025. ANDiE: McDannald et al., Appl. Phys. Rev. 9, 021408 (2022), doi:10.1063/5.0082956; and Neutron News 34, 6 (2023), doi:10.1080/10448632.2023.2190714.

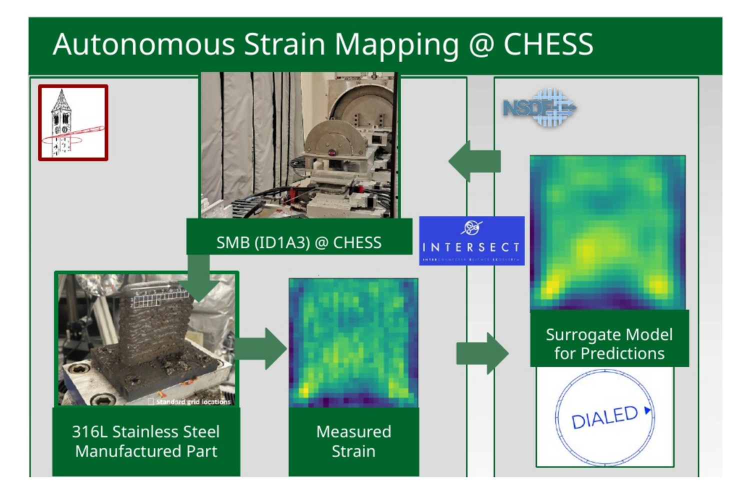
- Jun. 2026 — SNS NOMAD, automated "how long to measure."

  Neutrons are flux-limited, so counting time is the scarce resource: a live ADARA stream is reduced continuously, uncertainty in S(Q) is tracked against user criteria, and time-to-stop is predicted — the instrument stops and changes sample on its own. Demonstrated on diamond, graphite, and porous carbon; 1+ TB of streams saved for replay.

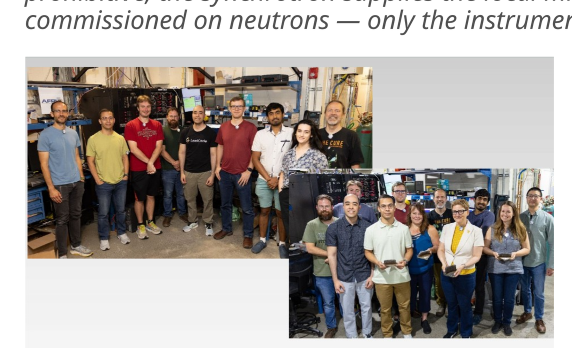
5. AUTONOMOUS X-RAY DIFFRACTION AT CHESS

Jun. 1–9, 2026 (setup Jun. 1–3; experiment Jun. 3–9) — Structured Materials Beamline (SMB / ID1A3), Cornell High Energy Synchrotron Source. The first INTERSECT autonomous scattering experiments outside ORNL, hosted on National Science Data Fabric infrastructure.

- Energy-dispersive XRD strain mapping of the same 316L stainless-steel thin walls (55 × 8 × 65 mm) measured during the VULCAN experiment. Measuring the full 1 × 1 mm grid would take ~1700 scans at ~90 s each; DIAL active learning instead picks the next gauge volume and returns a surrogate strain map, and the beamline SPEC control takes the next point.



Autonomous strain mapping at CHESS. Neutrons give the full 3D strain field but sub-mm resolution is time-prohibitive; the synchrotron supplies the local micromechanical view. Same DIAL service and strategy commissioned on neutrons — only the instrument changed.

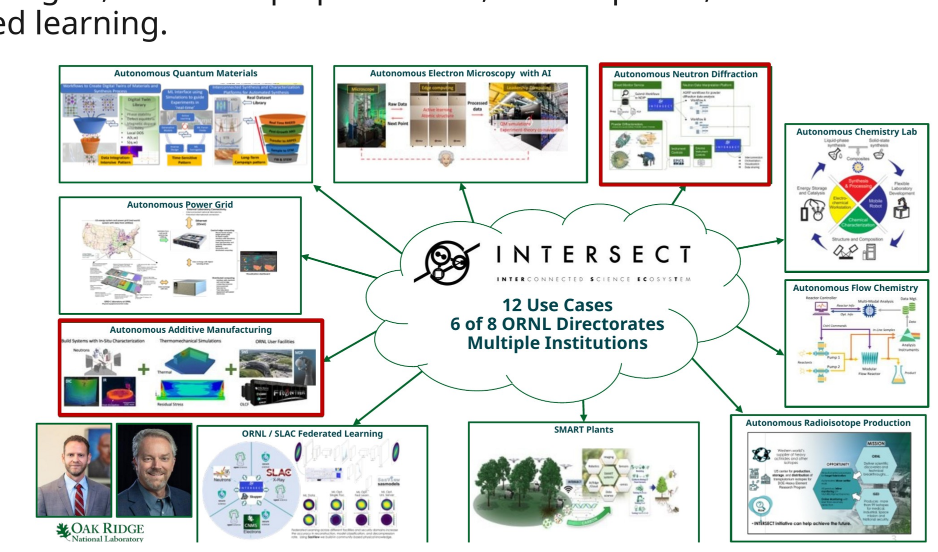


- Press:
  - ORNL, "AI powers self-driving science"
  - Cornell/CHESS, "Where the beam points next"
  - UTK, "A geographically distributed workflow"

ORNL | Cornell/CHESS | UTK

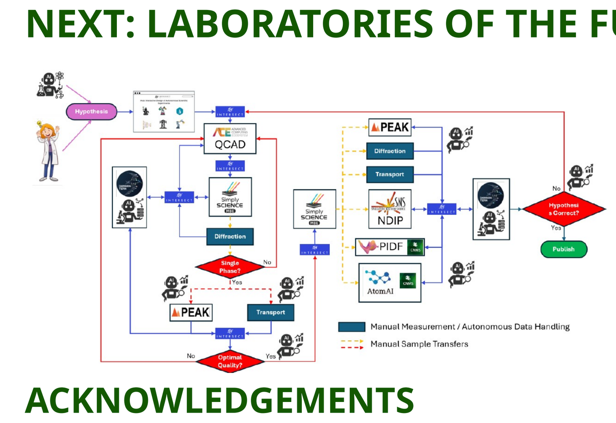
6. ACROSS THE ECOSYSTEM

The same SDK, core services and reusable capabilities also connect autonomous chemistry and flow chemistry, electron microscopy with AI, quantum materials, the power grid, radioisotope production, SMART plants, and ORNL/SLAC federated learning.



Shared capabilities cross domains: NDIP/Galaxy refinement workflows serve both the Autonomous Chemistry Lab and neutron diffraction, and DIAL steers x-rays, neutrons and 3D printers alike. Follow-on work continues in ILLUMINE (ASCR/BES), BRaVE (BES) and the DOE Genesis Mission.

NEXT: LABORATORIES OF THE FUTURE (LOTF)



Laboratories of the Future (LOTF) is ORNL's new five-year Director's R&D initiative: AI-enabled, closed-loop workflows linking experiment, data, models and decisions.

INTERSECT is the connective layer of the Jan.–Oct. 2026 ORNL pilot (left) — an end-to-end materials-by-design loop across 4 directorates, 10 divisions, OLCF, SNS and CNMS. MULTIBUS supports the pilot; the team is submitting to the open LOTF call.

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