



June 13, 2025 | A2SD Workshop

Scientific Labs of the Future: Creating an Ecosystem for Multi-Domain Science

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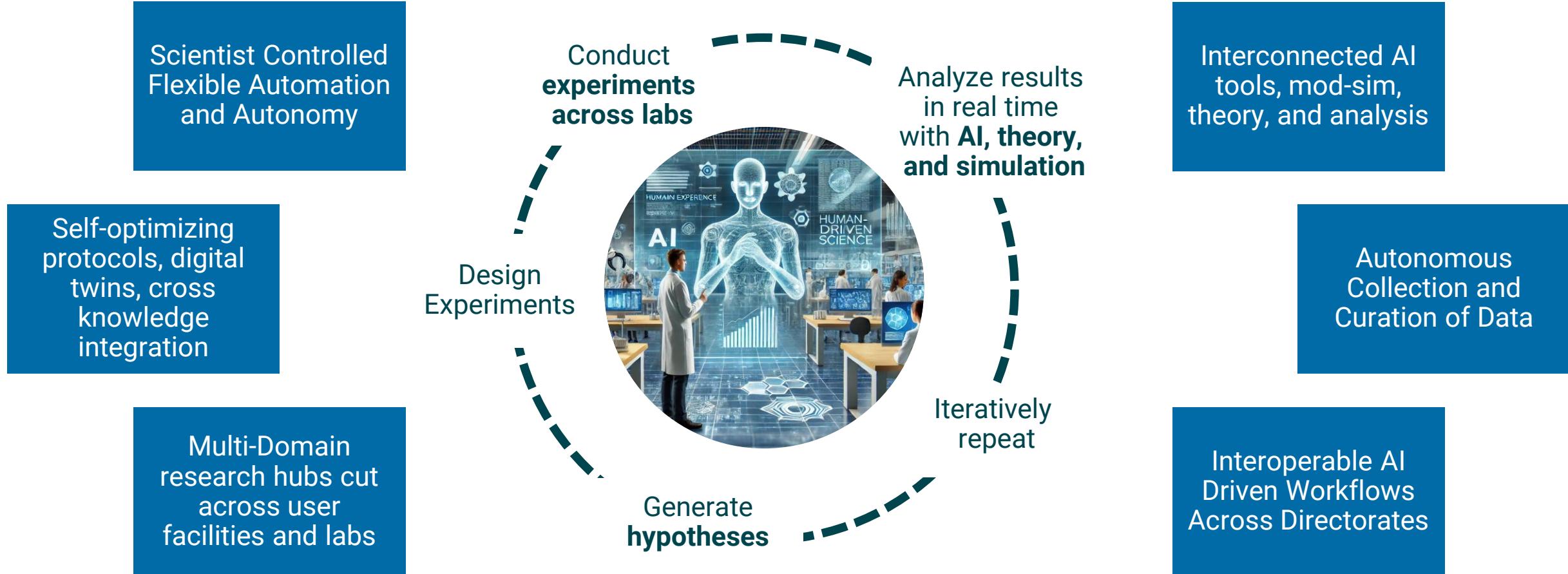


U.S. DEPARTMENT
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Smart Labs of the Future: AI-Orchestrated Autonomous and Connected Research Ecosystem

to accelerate advances that would have been otherwise impossible

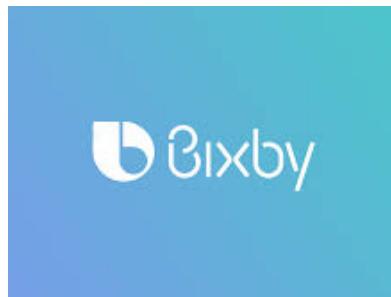


AI Agent drive autonomous experiments with
Humans in/on/out of the workflow loop

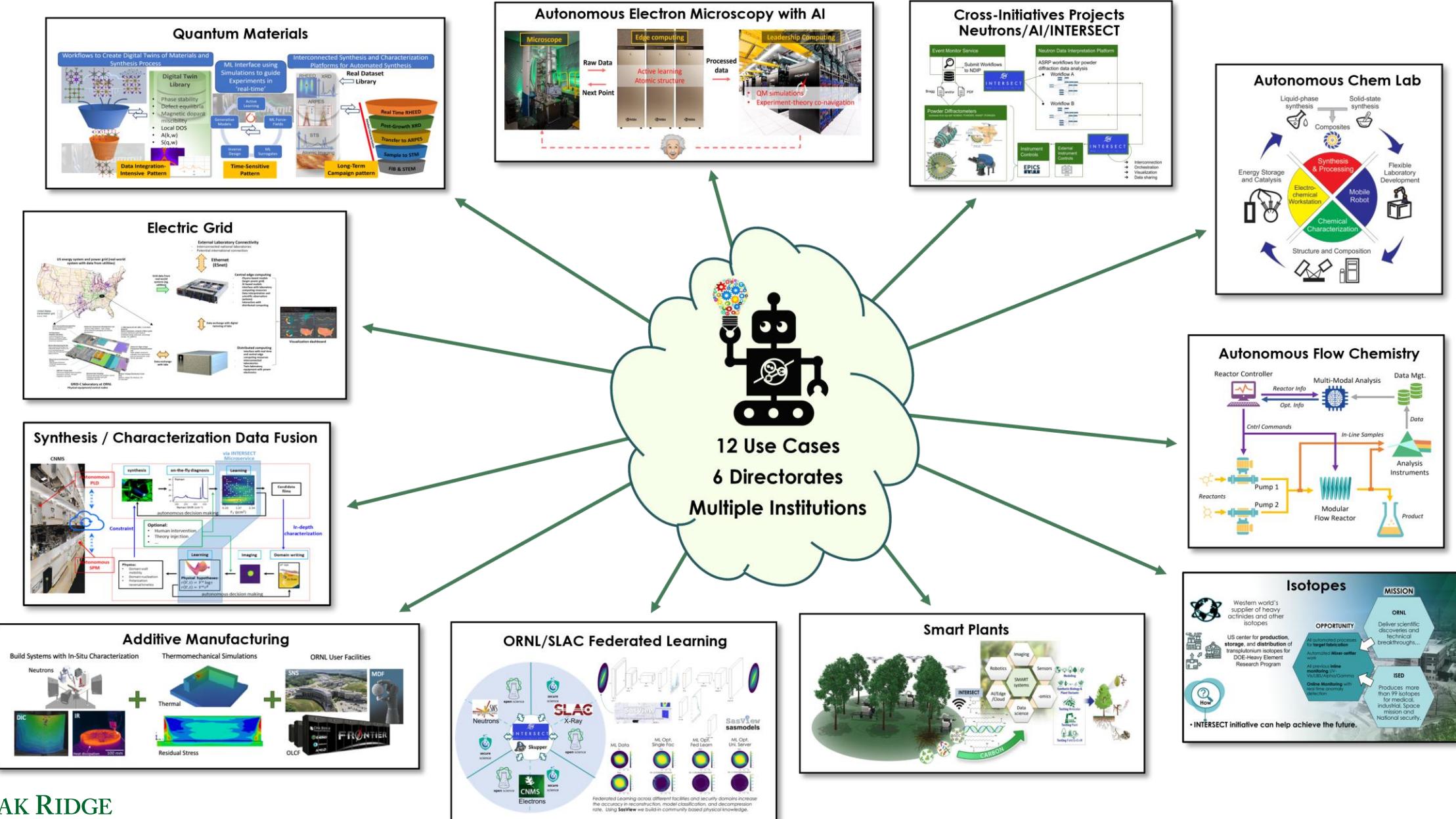
What We All Really Want



"Hey Oakley,
Help me solve a science problem!"

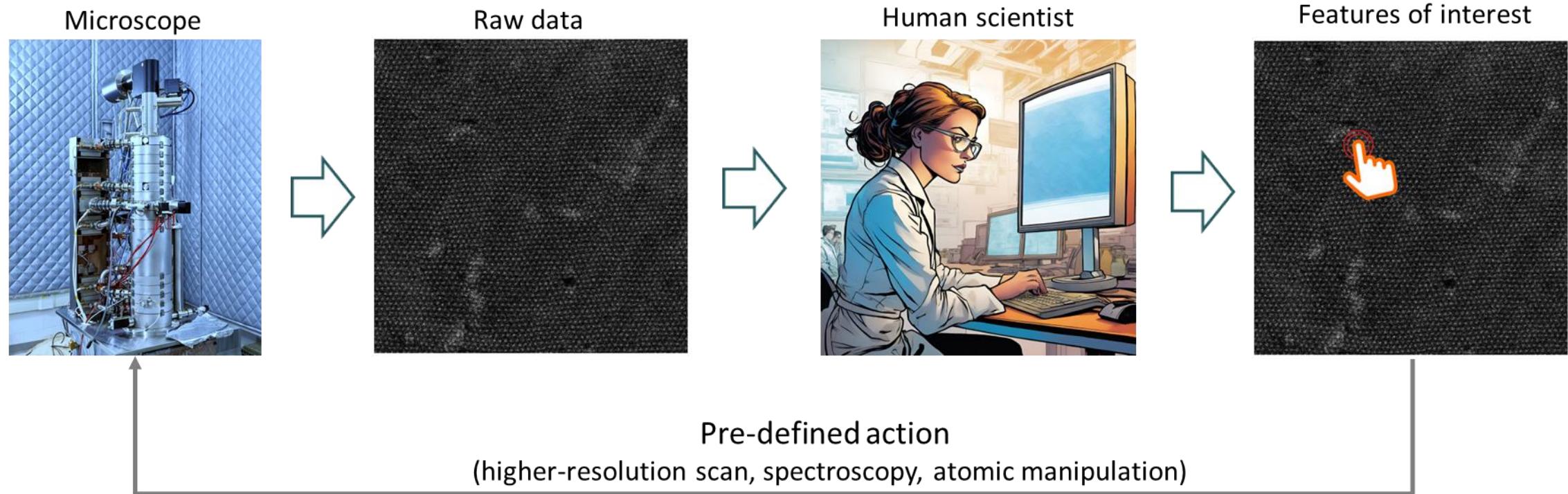


Ecosystem for Multi-Domain Science



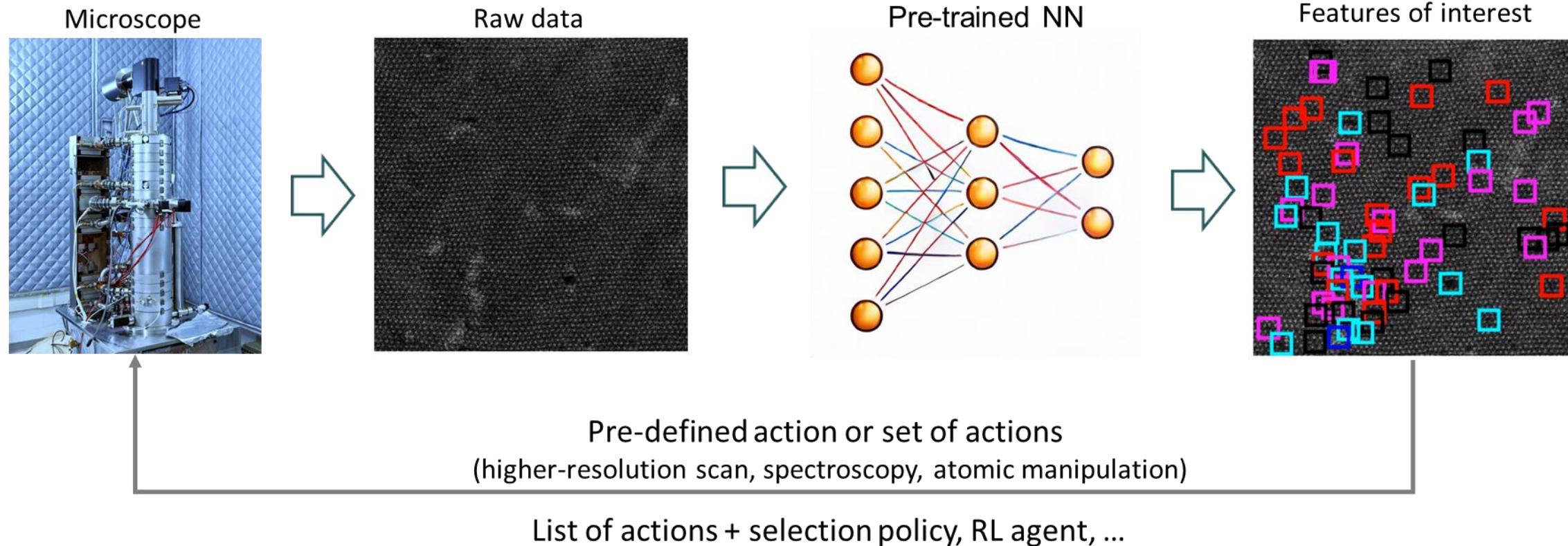
Autonomous Experiments in Electron Microscopy

First, let's revisit a standard human-centric workflow



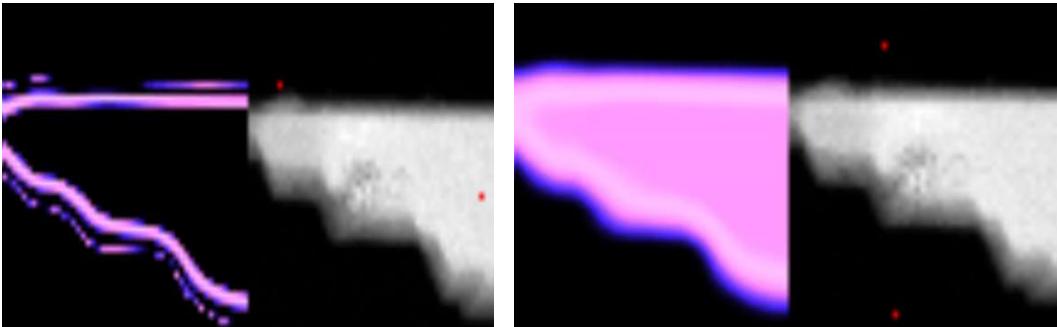
Autonomous Experiments in Electron Microscopy

Rapid object detection and action system (RODAS) - *a priori* defined objects of interest that can be recognized in real time with a pre-trained neural network.

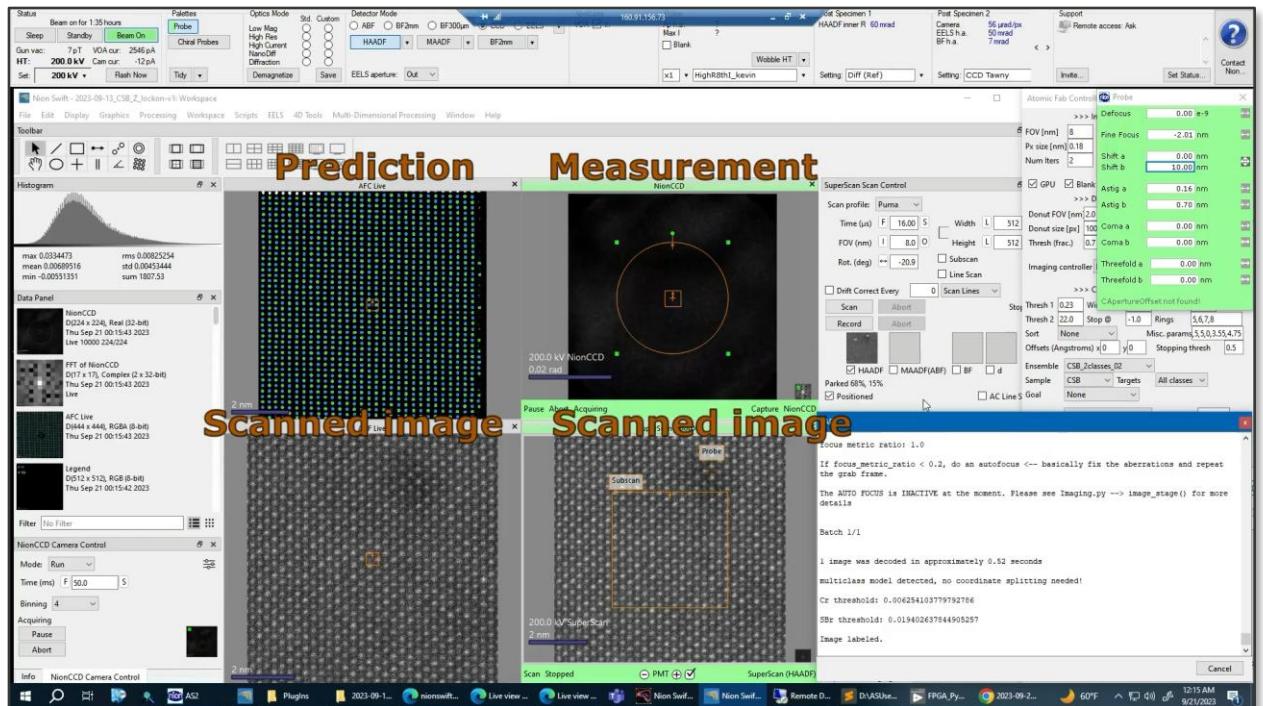


Autonomous Experiments in Electron Microscopy

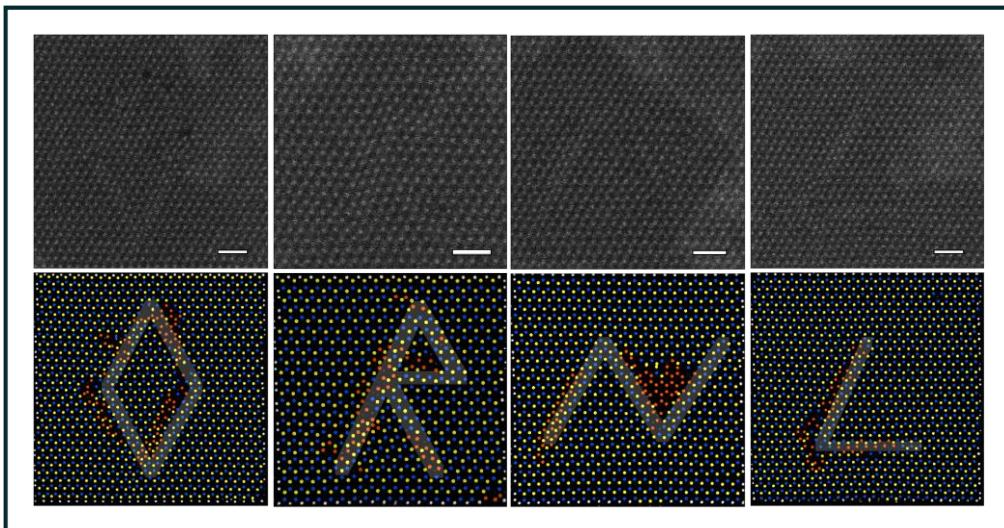
Discovering physics in a “new” material MnPS₃



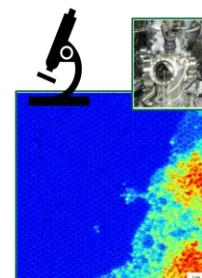
Discovering and classifying defects in materials



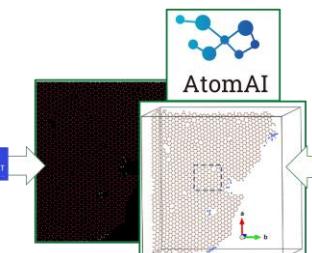
Controlling materials for tailored properties



Instrument



Edge



HPC



Additive Manufacturing – 3D Printing of Anything

AM: Building a part layer-by-layer by melting small amounts of powder/wire at a time

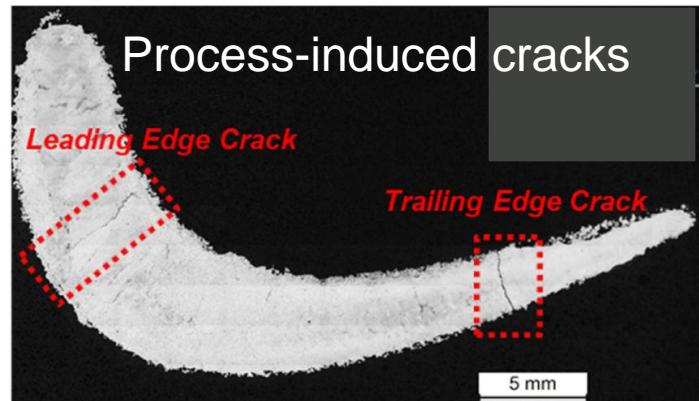
Potential for new, complex part topologies and optimized, location-specific material properties

A difficulty...

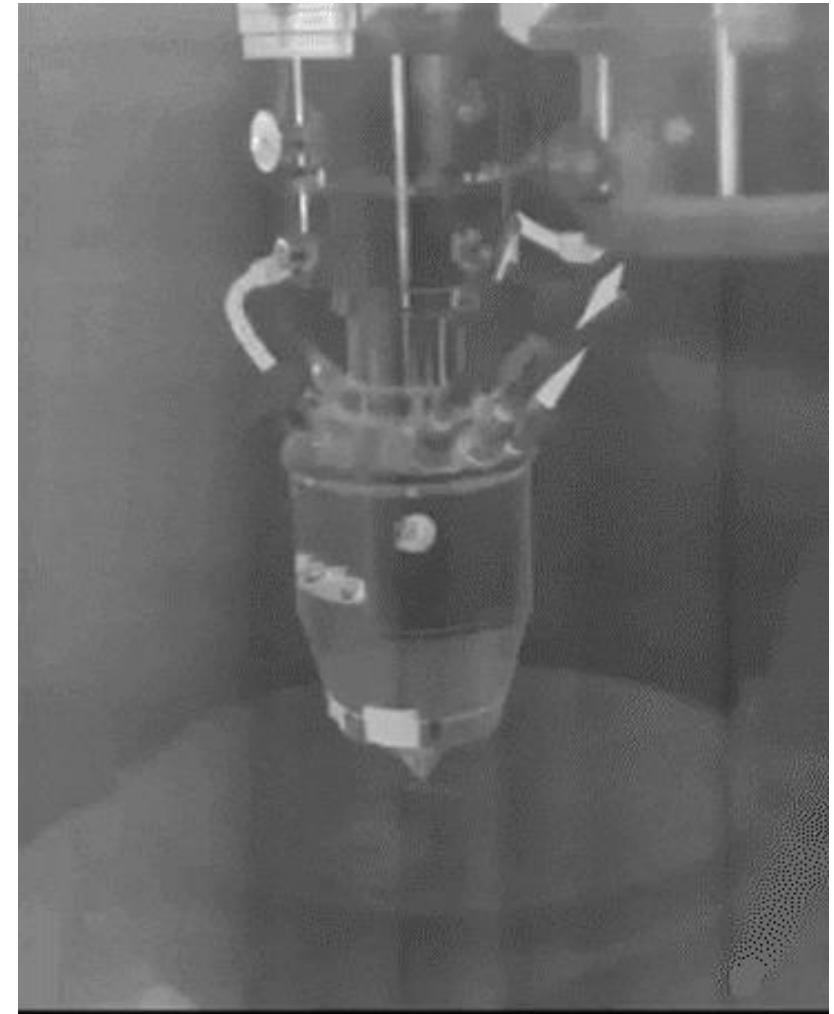
Part quality is sensitive to process parameters



Any change can require unintuitive process changes

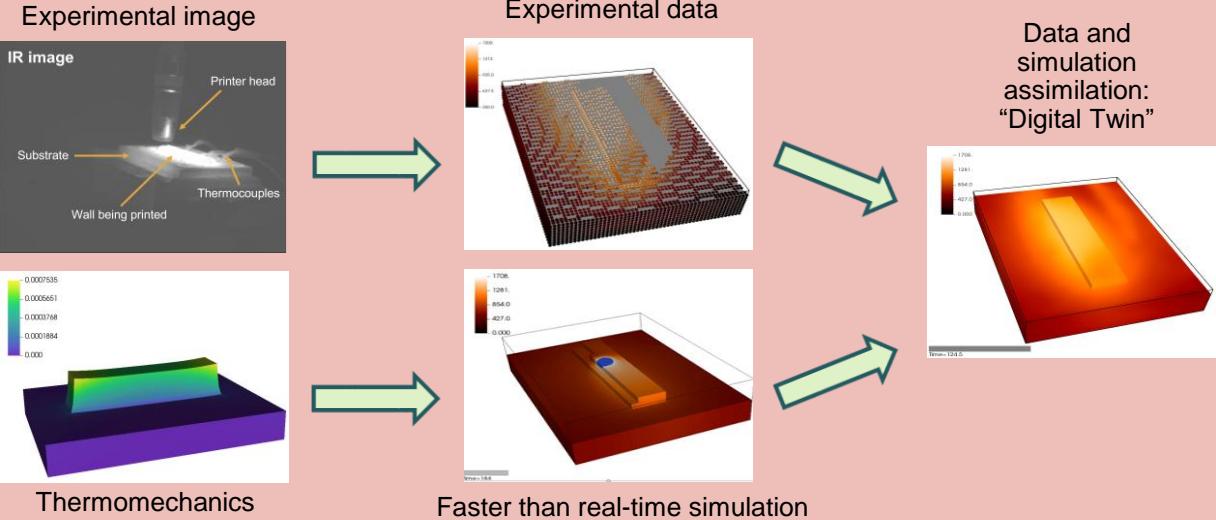


Lee, et al, Additive Manufacturing, 2020.

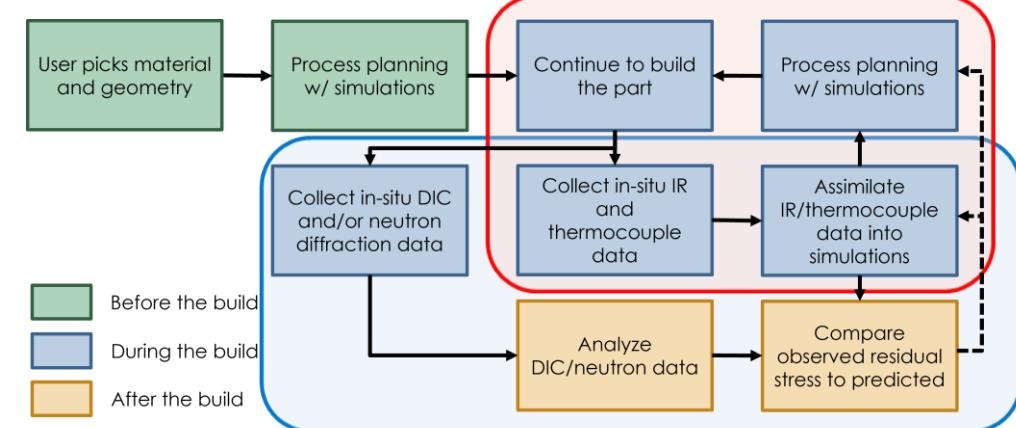


The Power of an Ecosystem – Interoperability and Reuse

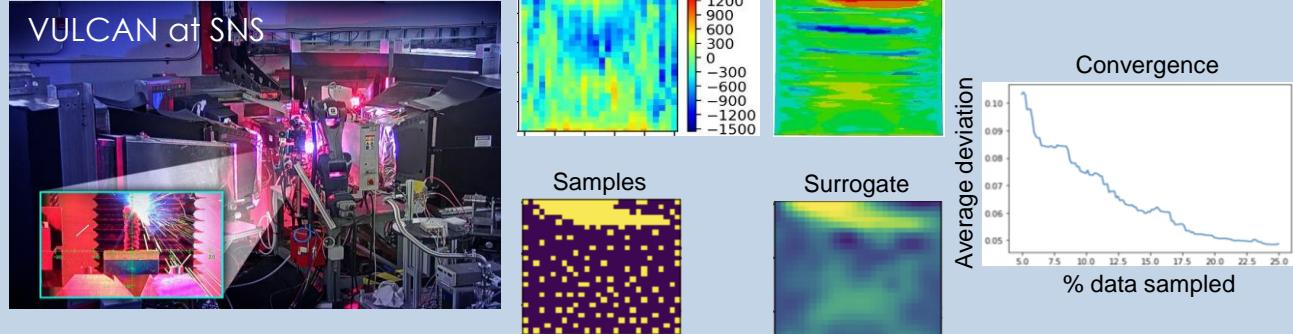
Additive Manufacturing Digital Twin



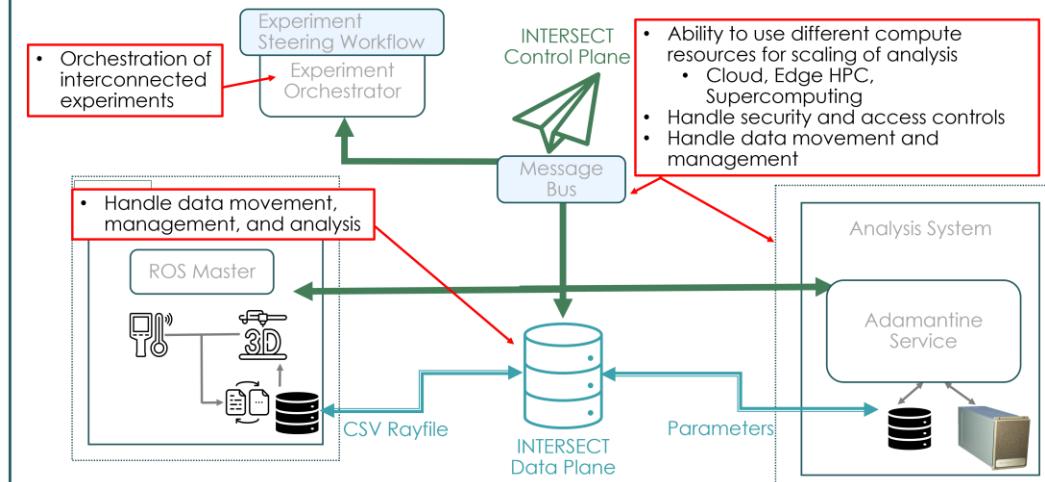
Additive Manufacturing Autonomous Workflow



Additive Manufacturing / SNS Integration

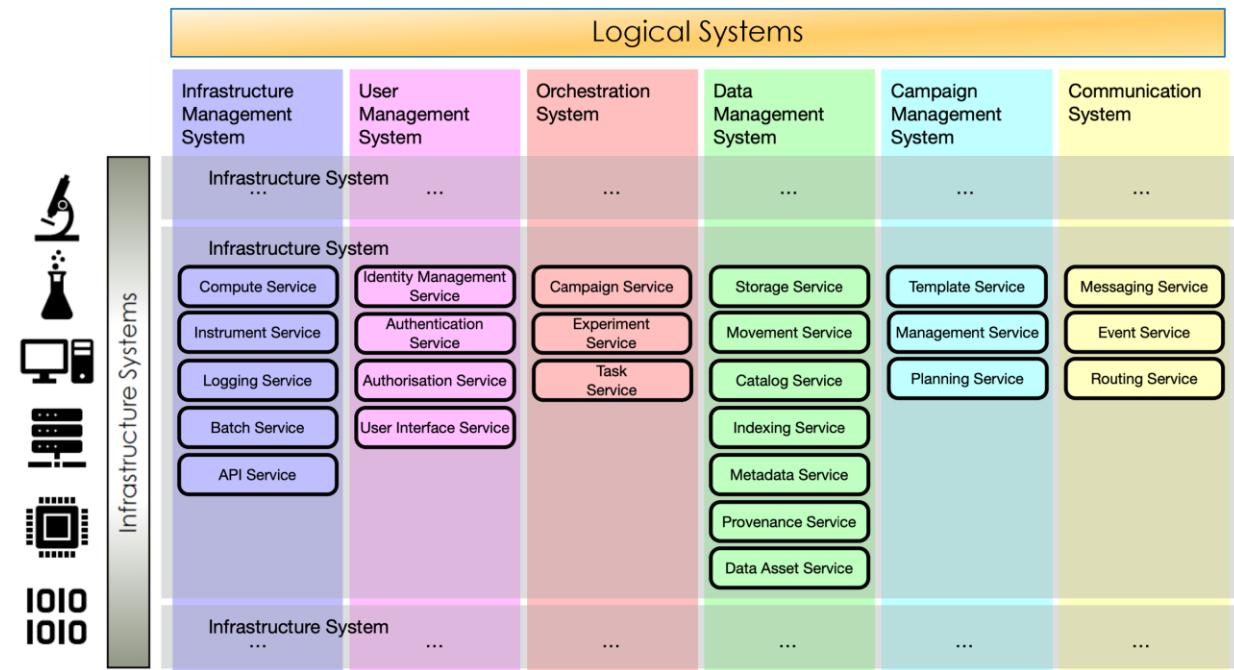
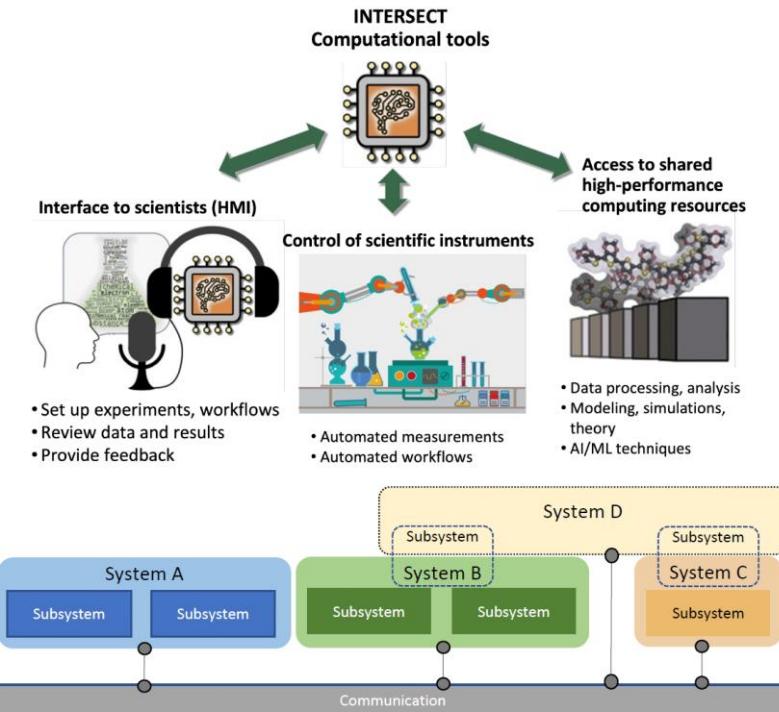


INTERSECT Software Services



Systems of Systems Architecture

Break the experimental tasks down into the smallest components. Treat the components as a system and figure out how to connect them in the simplest ways.



- Simple minded systems: Infrastructure Systems and Logical Systems
- Microservices provides the links which creates capabilities
- Capabilities and connections between Infrastructure and Logical systems enabled by communications via simple message passing

Open Software

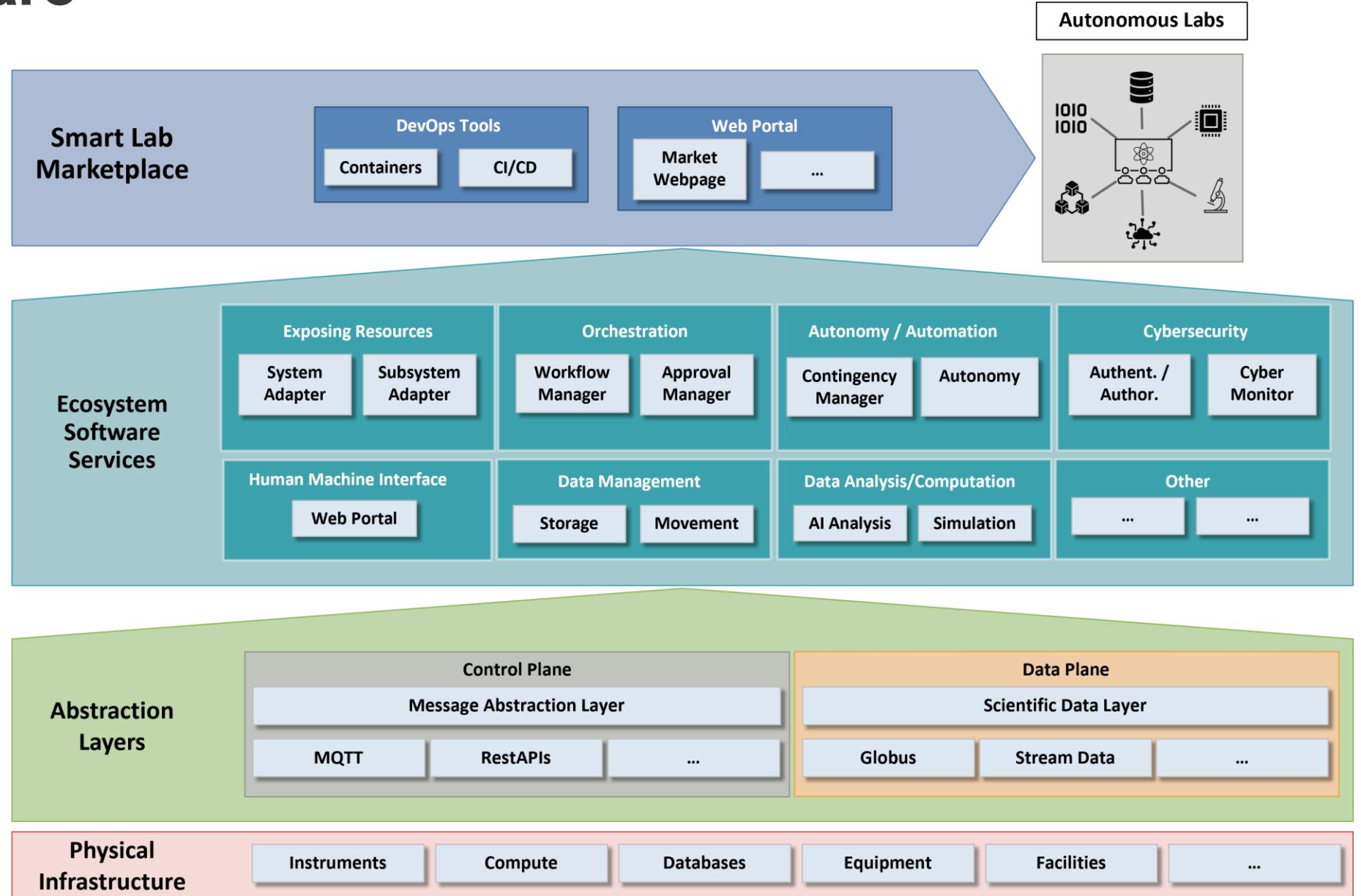
Rapid Deployment



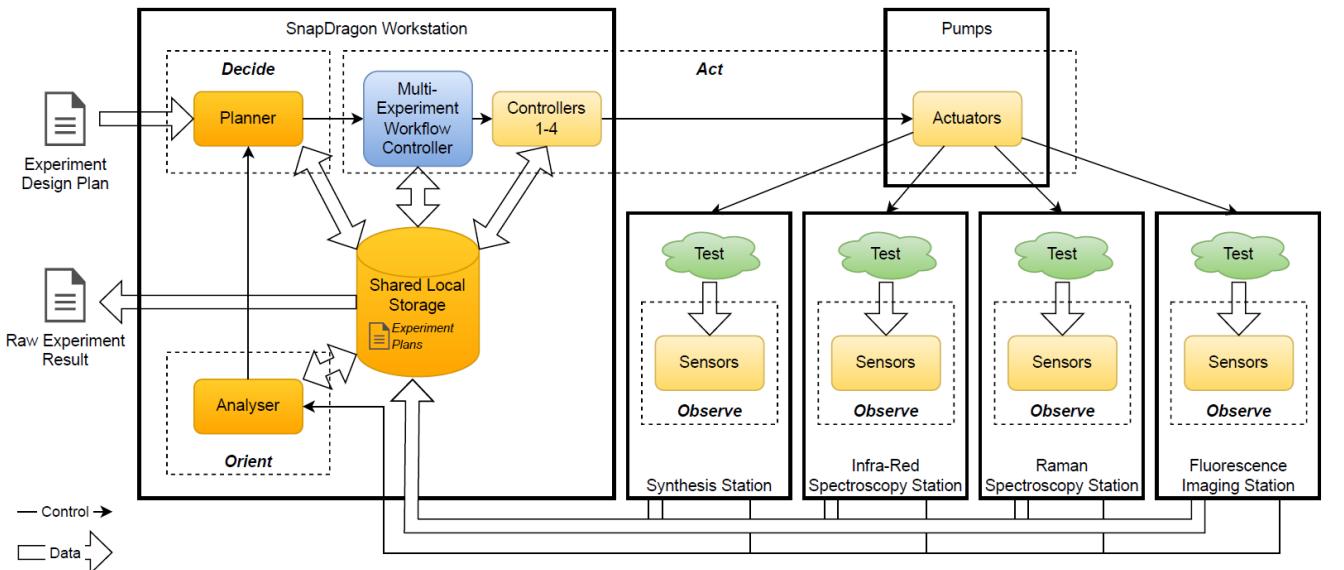
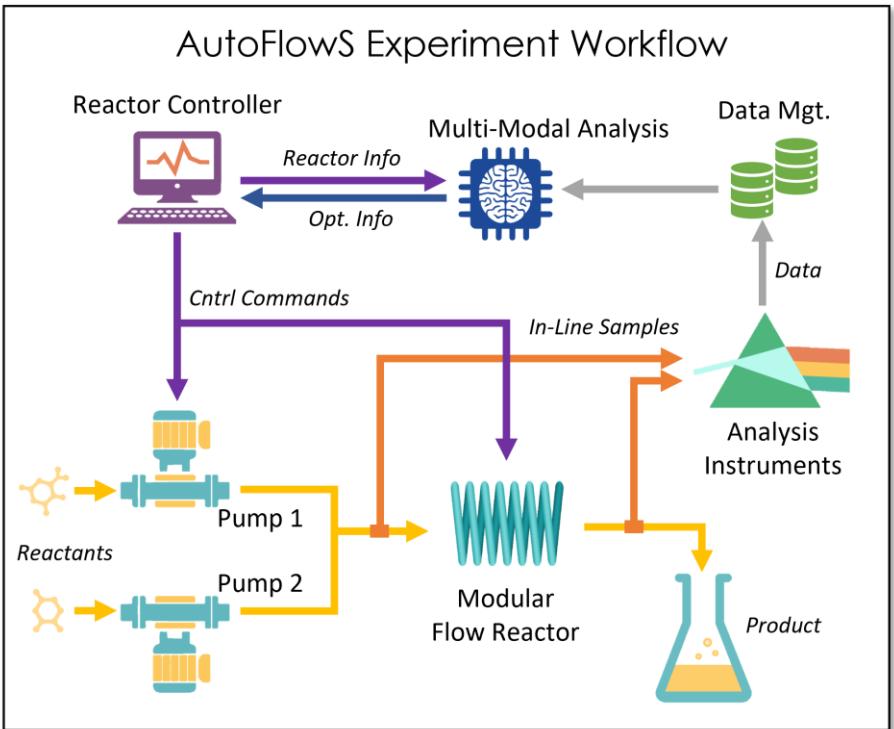
Flexibility and Reconfigurability



Interoperability



A Co-Design Approach



- Requires plug-n-play capabilities as the synthesis chamber and analysis capabilities changes depending on chemistry
- Requires multi-dimensional datasets for AI/ML training
- Requires workflow agent to connect with HPC (high performance computing) or edge computing (DGX box) depending on chemistry



Incorporating LLMs

- Gradient copolymers offer unique properties but challenging chemical synthesis
- Created database with 5823 copolymerization reactions based on literature and MD simulations
- Incorporated FORGE, ORNL's LLM, plus RAG into Autoflows workflow and add chemical thermodynamics model to direct and validate gradient copolymer production
- Scientist in the loop autonomous workflow combining LLM with MD simulations and flow reactor with multi-modal analysis



suggest synthesis recipe for 5-(tert-butoxycarbonyl)amino-1-pentanol

Based on the provided patent references, a possible synthesis recipe for 5-(tert-butoxycarbonyl)amino-1-pentanol is as follows:

Synthesis recipe for 5-(tert-butoxycarbonyl)amino-1-pentanol:

Product: 5-(tert-butoxycarbonyl)amino-1-pentanol
Yield: 92-76%

Reaction SMILES: NCCCCO.CC(C)(C)OC(=O)OC(=O)OC(C)C>CC(C)(C)OC(=O)NCCCCO

Reaction Description:

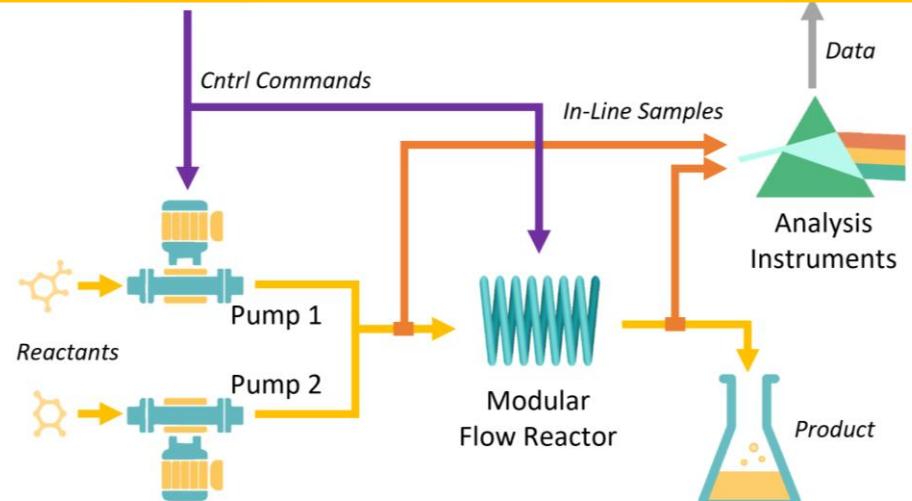
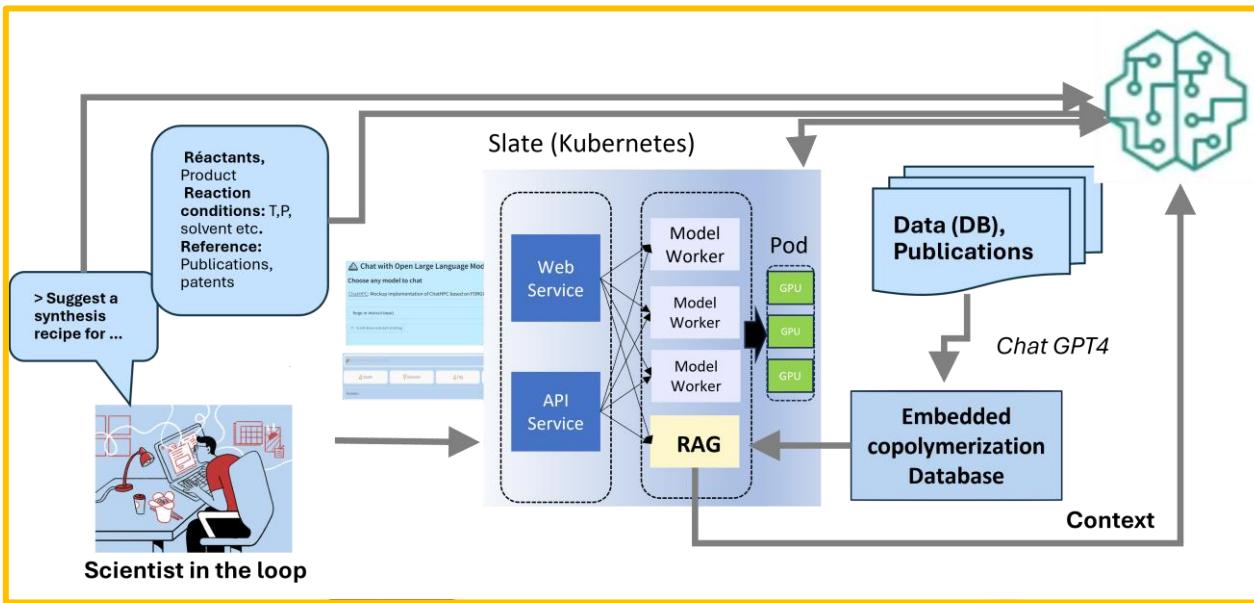
To a solution of 5-aminopentanol (1 g, 9.7 mmol) in CH₂Cl₂(100 mL) was added triethylamine (1.5 mL, 10.7 mmol, 1.1 equiv.) and the solution was cooled down to 0°C with an ice bath. Di-tert-butyl dicarbonate (2.11 g, 9.7 mmol, 1 equiv.) was added portion-wise and the solution was allowed to warm to RT and stir overnight at RT. The reaction completion was monitored and the reaction was added silica and the solvent was evaporated. The residue was purified by silica gel chromatography (CH₂Cl₂/MeOH 4% to 6%) to afford 5-(tert-butoxycarbonyl)amino-1-pentanol in 92-76% yield.

Reactant: 5-Amino-1-pentanol

Reaction Condition 1:

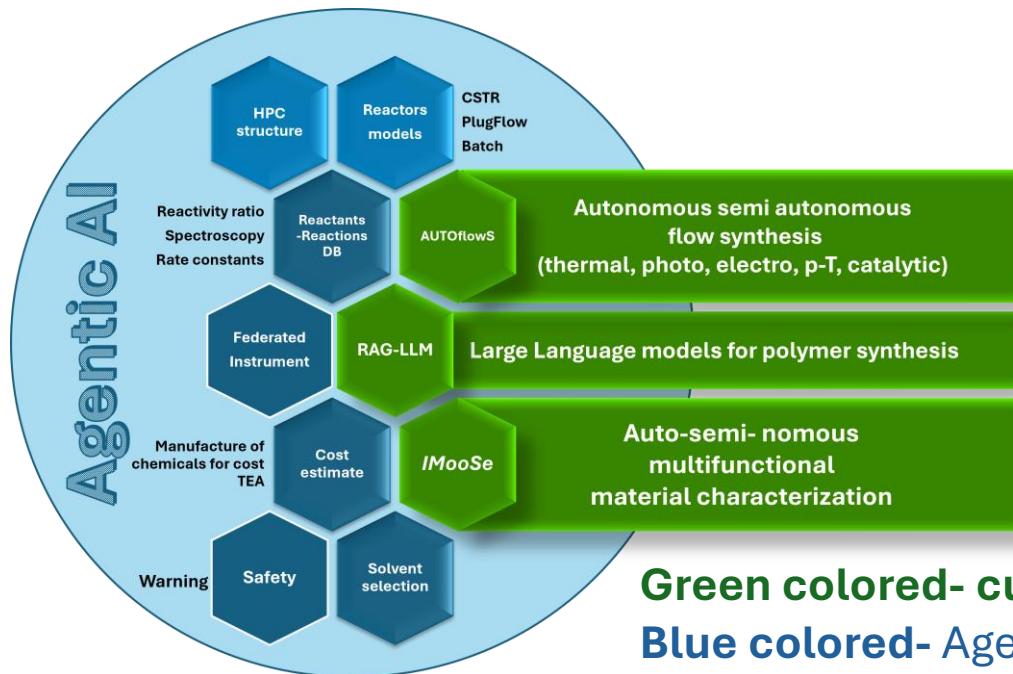
- Solvent: CH₂Cl₂

Example Result



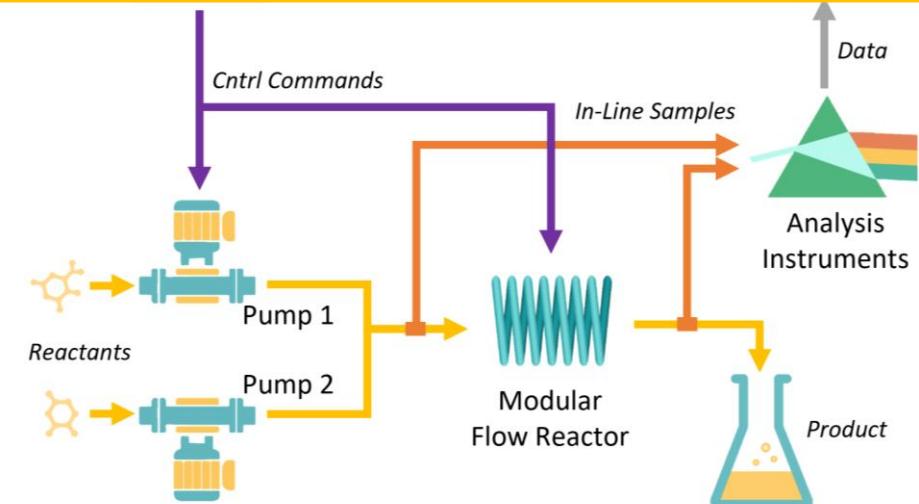
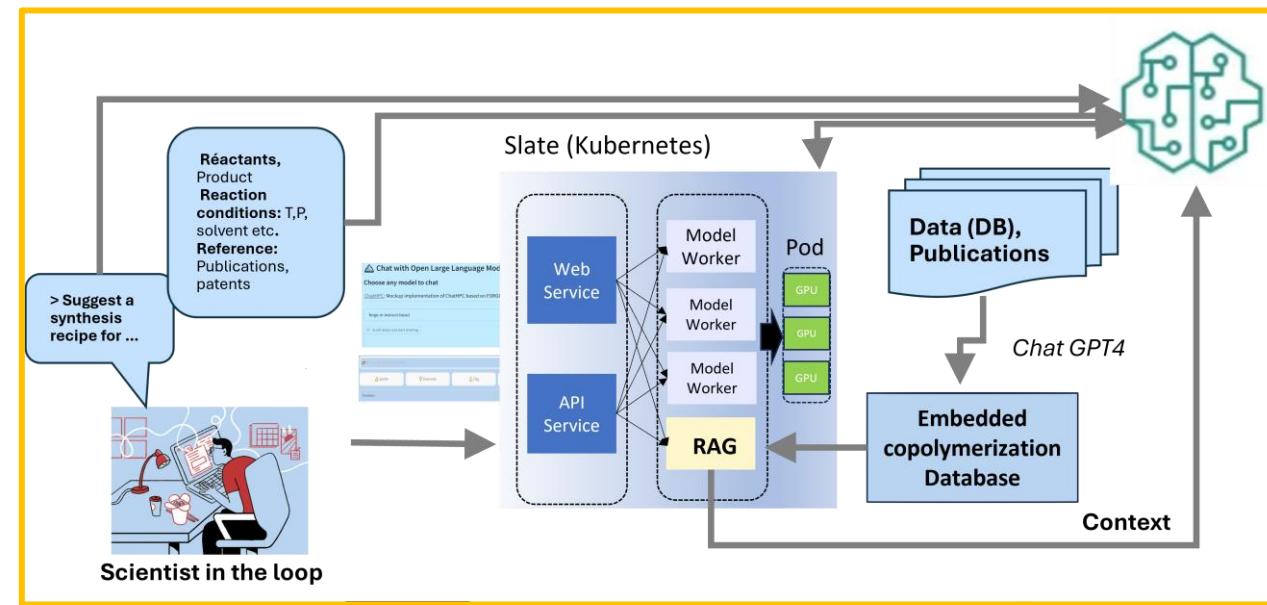
Towards Agentic AI

- Developing Agentic AI Agents to direct and control workflow with scientists in the loop
- Combines distributed synthesis, RAG-LLM and Agentic AI for synthesis of multifunctional polymers for AM
- Multiple AI Agents integrated into Federated HUB to tackle: modeling of reaction in complex configuration, Safety of reactions, MD simulation, multimodal testing

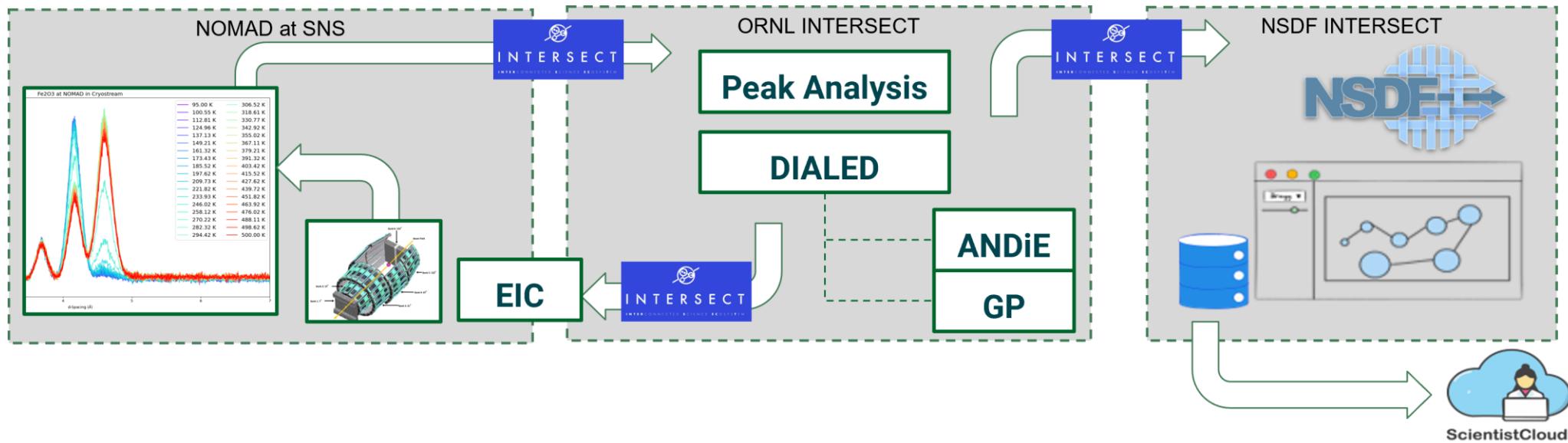


Green colored- current Agents

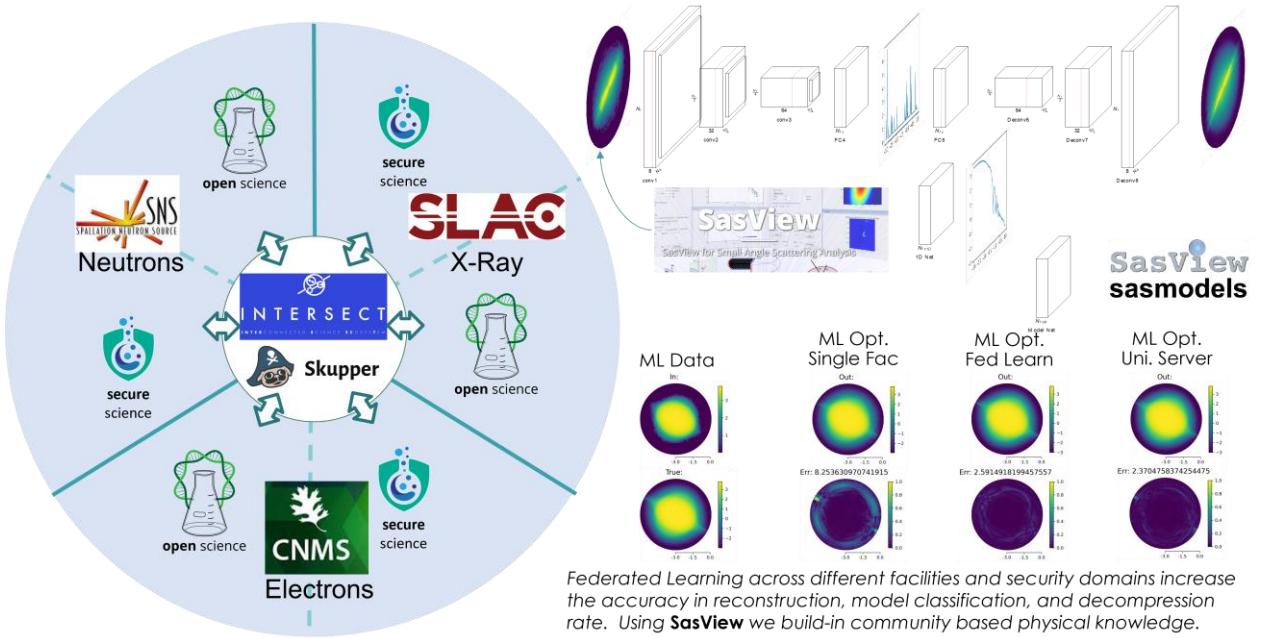
Blue colored- Agents being developed in collaboration with University of Tennessee, Georgia Institute of Technology



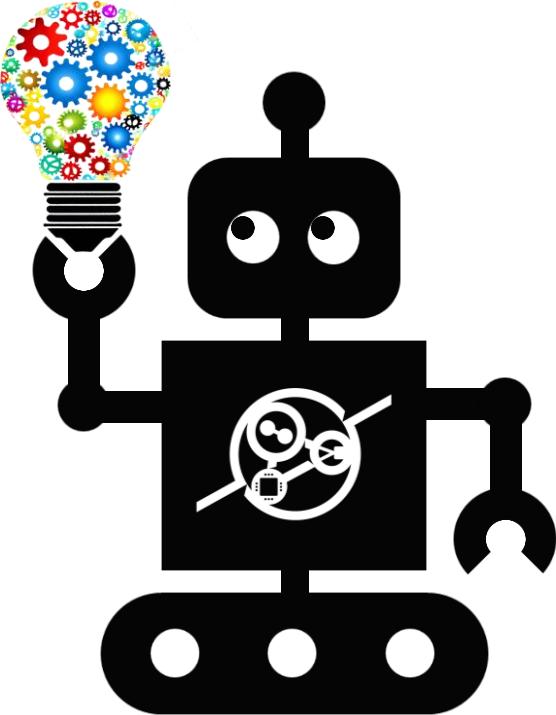
Beyond ORNL Borders



- (Top): Autonomous collection and analysis of neutron diffraction data(NOMAD at SNS) utilizing National Science Data Fabric (NSDF) **(ORNL/UTK/NIST/NSDF)**
- (Right): Federated Learning for Small Angle Scattering (SAS) Experimental Facilities **(IBM/ORNL/RedHat/SLAC)**



Questions?



INTERSECT Website:

<https://www.ornl.gov/intersect>

Architecture Documentation:

<https://intersect-architecture.readthedocs.io/en/latest/>

Architecture github repository:

<https://github.com/ORNL/intersect-architecture>

Software Development Kit website:

<https://intersect-python-sdk.readthedocs.io/en/latest/>

SDK github repository:

<https://github.com/INTERSECT-SDK/python-sdk>