OAK RIDGE National Laboratory

INTERSECT

INTERCONNECTED SCIENCE ECOSYSTEM

Rob Moore

INTERSECT Co-Director

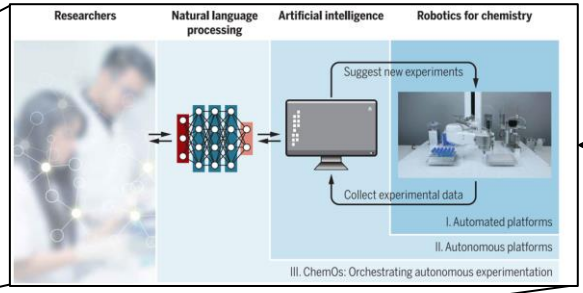
October 2, 2024

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

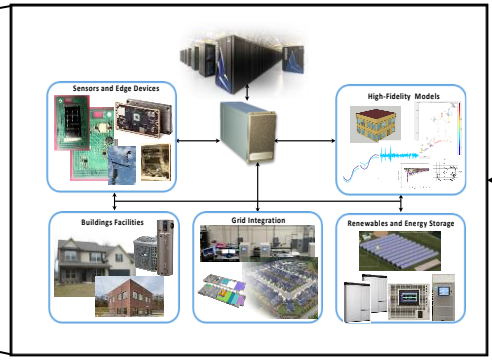
U.S. DEPARTMENT OF ENERGY

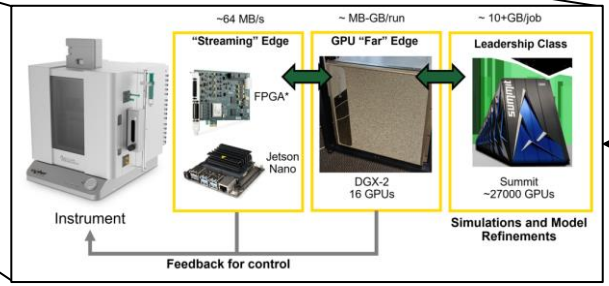
Smart Labs of the Future (2030+)

Materials Lab



Electric Grid Lab





Microscopy Lab

Interconnected Smart Labs

Interoperable Ecosystem is Required

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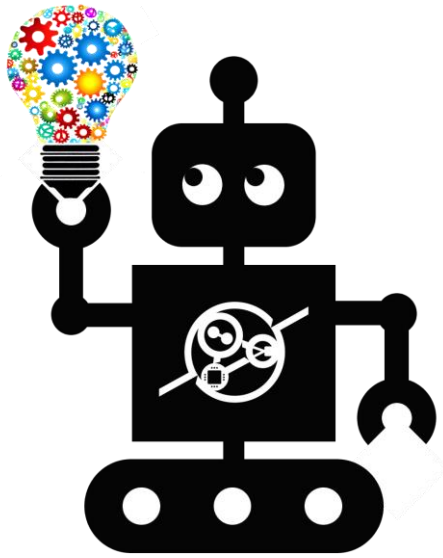
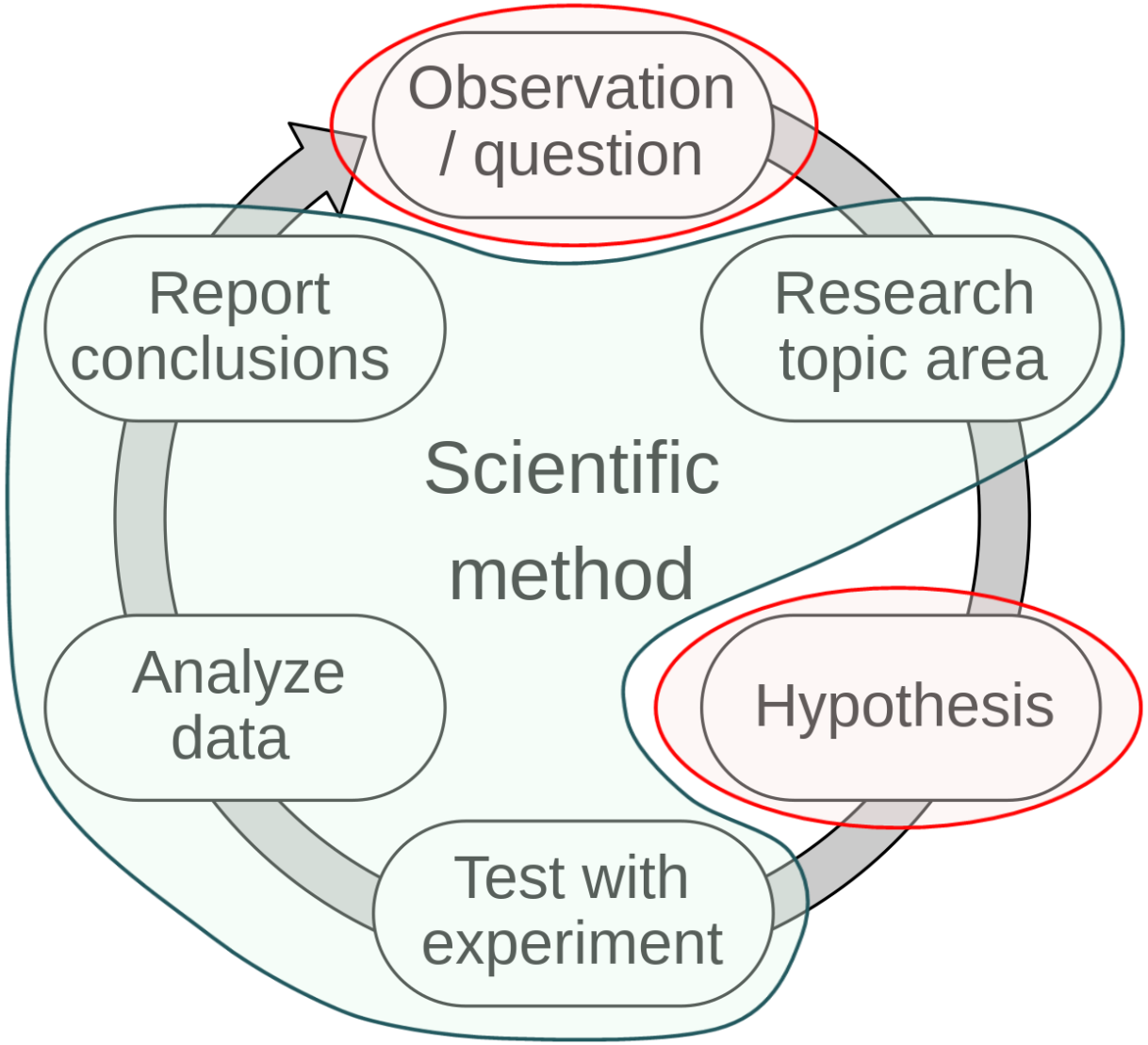
Let's start someplace that we can all understand





What We All Really Want

Hey Google

alexa

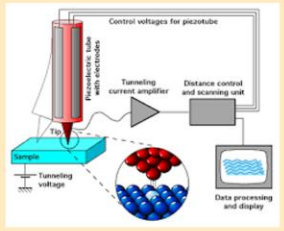
Siri

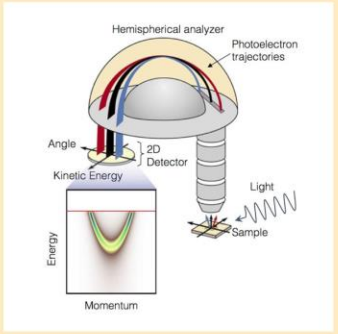
"Hey Oakley,
Help me solve a science problem!"

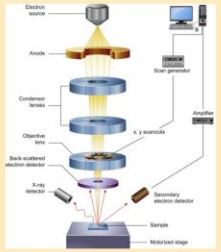
Bixby

INTERSECT – Connecting the Pieces

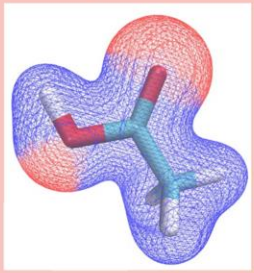
Characterization

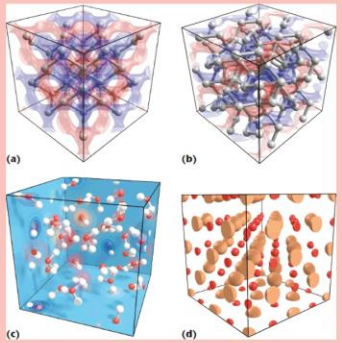






Theory





Simulation

AI Algorithms

nD Data

ML Descriptor

Edge Computing

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Edge Computing

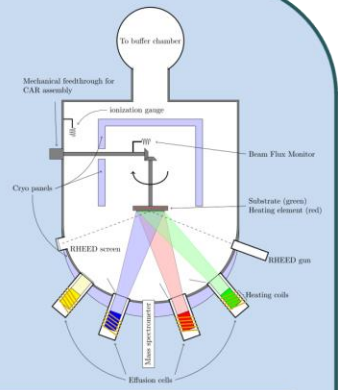
Growth Parameter

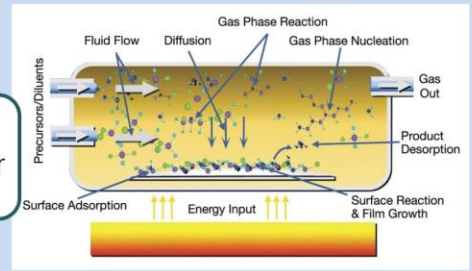
Orchestration, Workflow

Communication

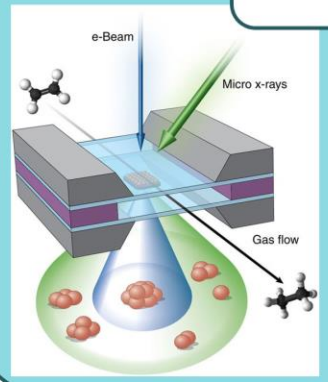
Fabrication

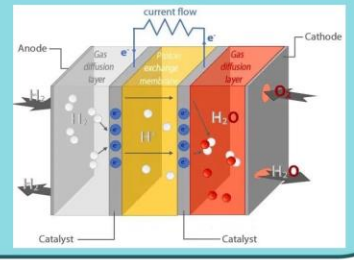
Synthesis





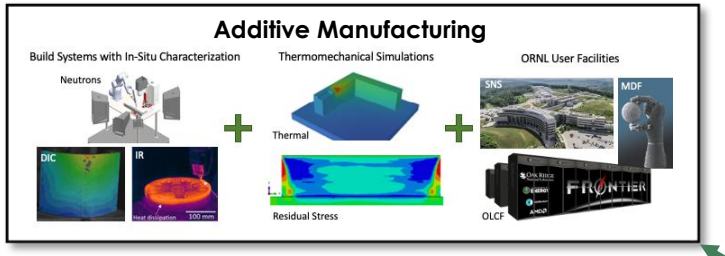
in operando, proof of principle

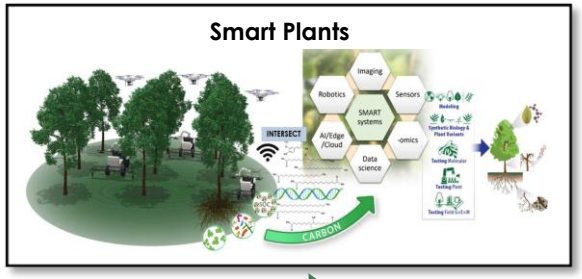


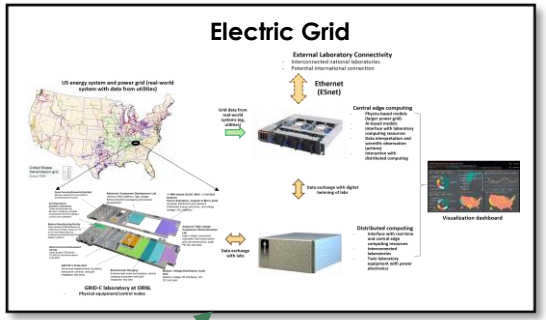


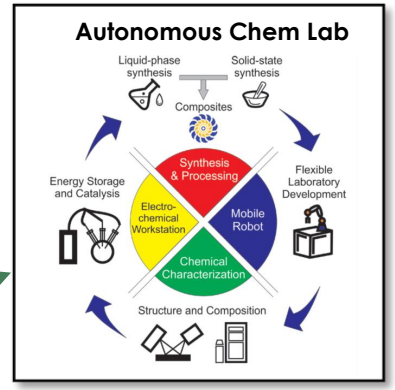
Automation

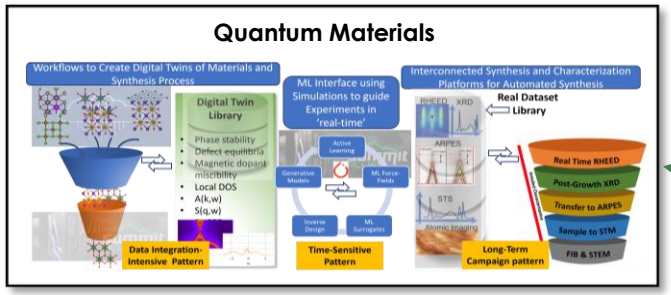
INTERSECT Use Cases

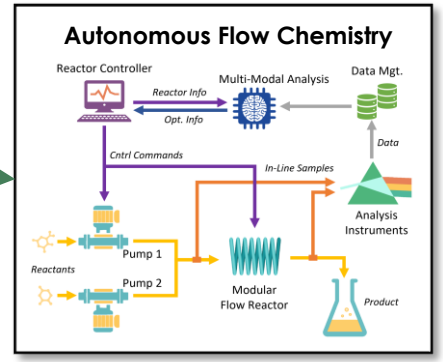


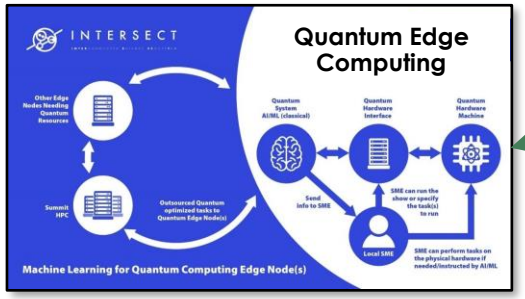


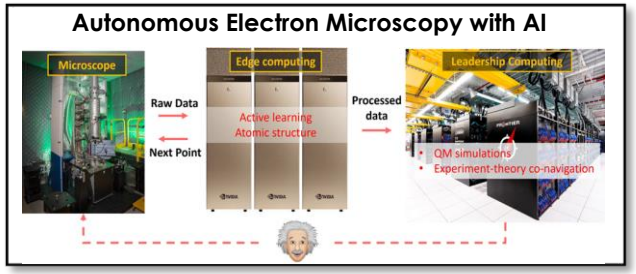


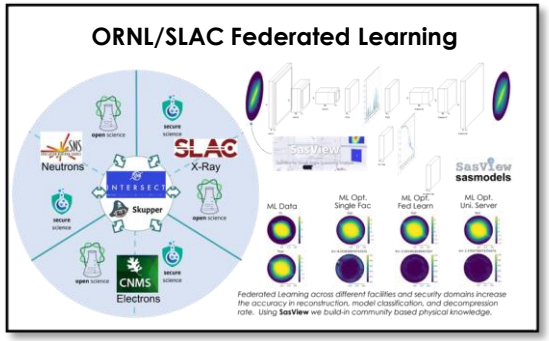


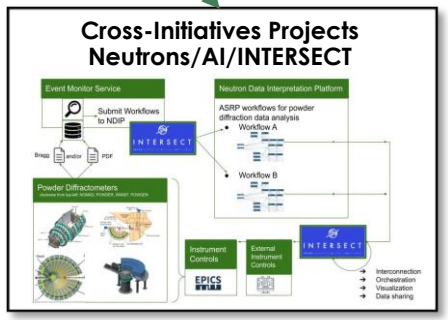


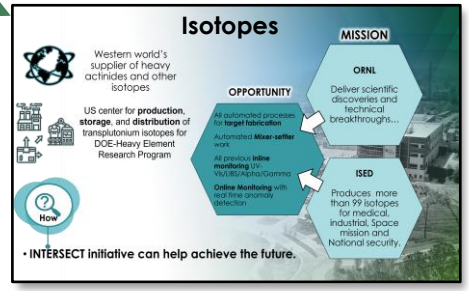












11 Use Cases

6 Directorates

Multiple Institutions

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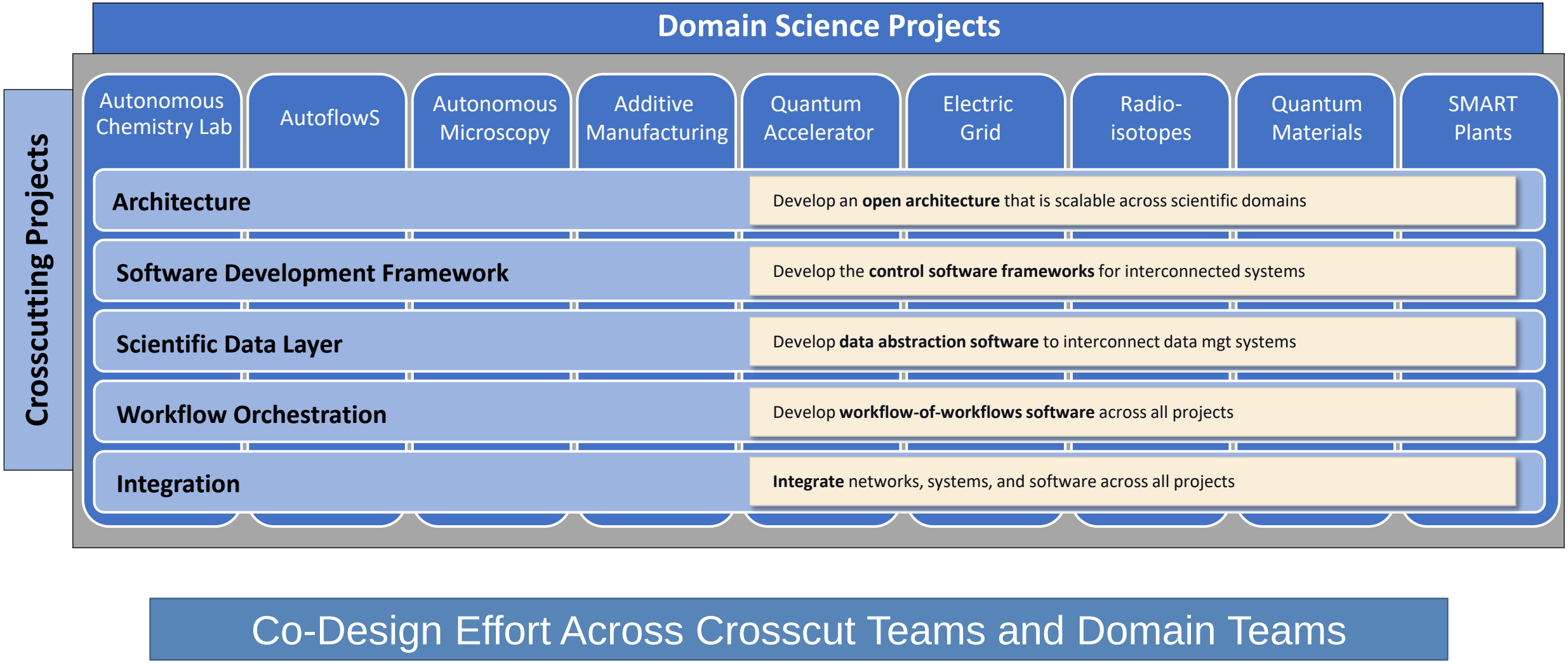
INTERSECT Programmatic Structure



Co-Design Effort Across Crosscut Teams and Domain Teams

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INTERCONNECTED SCIENCE ECOSYSTEM

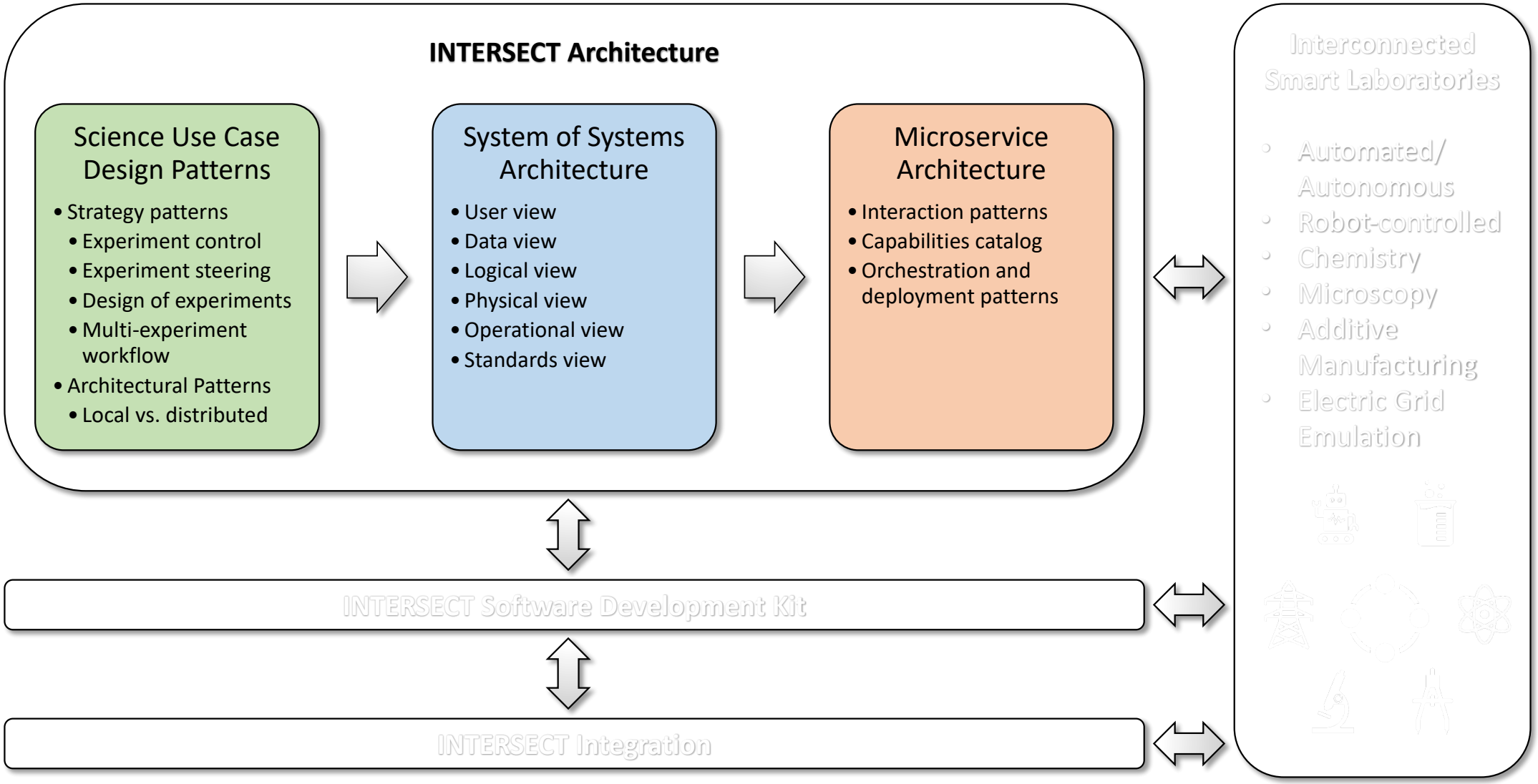
INTERSECT

INTERCONNECTED SCIENCE ECOSYSTEM

Co-Directors: Ben Mintz and Rob Moore

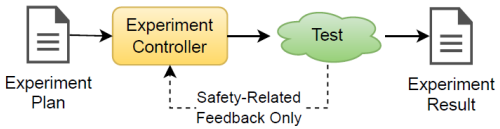
Cross-cut	*Architecture*	**Christian Engelmann**, Olga Kuchar, Swen Boehm, Michael Brim, Kack Lange, Thomas Naughton, Patrick Widener
	Software Development Kit	**Addi Malviya Thakur**, Seth Hitefield, Marshall McDonnell, Matthew Wolf, Richard Archibald, Lance Drane, Jesse McGaha, Robert Smith, Gavin Wiggins, Joel Ewan, Michael Brim, John Hetrick, Mark Abraham, Sergey Yakubov, Greg Watson, Ben Chance, Clara Nguyen, Matthew Baker, Robert Michael
	Integration	**Nageswara Rao**, Ramanan Sankaran, Anees Al Najjar, Helia Zandi, Susan Hicks
	Scientific Data Layer	**Swen Boehm,** Patrick Widener, Dale Stansberry, Seth Hitefield, Christian Engelmann, Olga Kuchar
	Orchestration	**Renan Souza,** Tyler Skluzacek, Frederic Suter, Mark Coletti, Rafel Ferreira da Silva, Olga Kuchar
Science Domains	*Quantum Acceleration*	**Christopher Seck**, Giles Buchs, Jiafeng Cui, Thomas Naughton, Amir Shehata, In-Saeng Suh, Nicholas Peters
	Autonomous STEM	**Debangshu Mukherjee**, Ayana Ghosh, Jacob Hinkle
	Additive Manufacturing	**Stephen DeWitt**, Bruno Turcksin, James Haley, Yousub Lee, Thomas Feldhausen, Ke An, Ayana Gosh, Singanallur Venkatakrishnan
	Grid	**Suman Debnath**, Harry Hughes, Jongchan Choi, Phani Marthi, Steven Hahn, Qianxue Xia, Kuldeep Kurte
	Autoflows	**Rigoberto Advincula**, Bobby Sumpter, Kunlun Hong, Rama Vasudevan, Ilia Ivanov
	Autonomous Chem Lab	**Sheng Dai**, Craig Bridges, Ilja Popovs, Bobby Sumpter, Tolga Aytug, Huimim Luo, Andrzej Nycz
	SMART Plants	**Udaya Kalluri**, Peter Wang, Andrzej Nycz, Kenneth Howe
	Quantum Materials	**P. Ganesh**, Debangshu Mukherjee, Ayana Ghosh, Matthew Brahlek, Peter Doak, Thomas Maier, Addis Fuhr
	Isotopes	**Punam Thakur**, Christopher Greulich, Santa Jansone-popova, Stacy Queern, Luke Sadergaski, Dongwan Shin, Brad Skidmore

Build from the Ground Up with Uniform Standards



Use Case Design Pattern Strategy

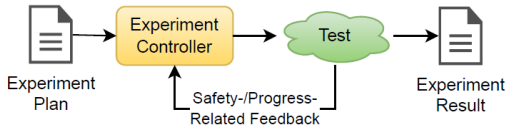
Experiment Control



Executes an existing plan

- Open loop control
- Automated operation

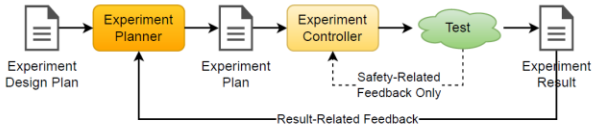
Experiment Steering



Executes an existing plan, depending on progress

- Closed loop control
- Autonomous operation
- Extends patterns:
  - Experiment Control

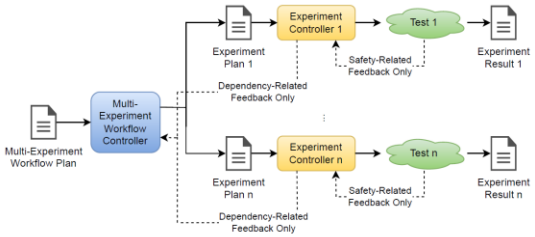
Design of Experiments



Creates / executes a plan, based on prior result

- Closed loop control
- Autonomous operation
- Use patterns:
  - Experimental Control
- May use patterns:
  - Experimental Steering

Multi-Experiment Workflow

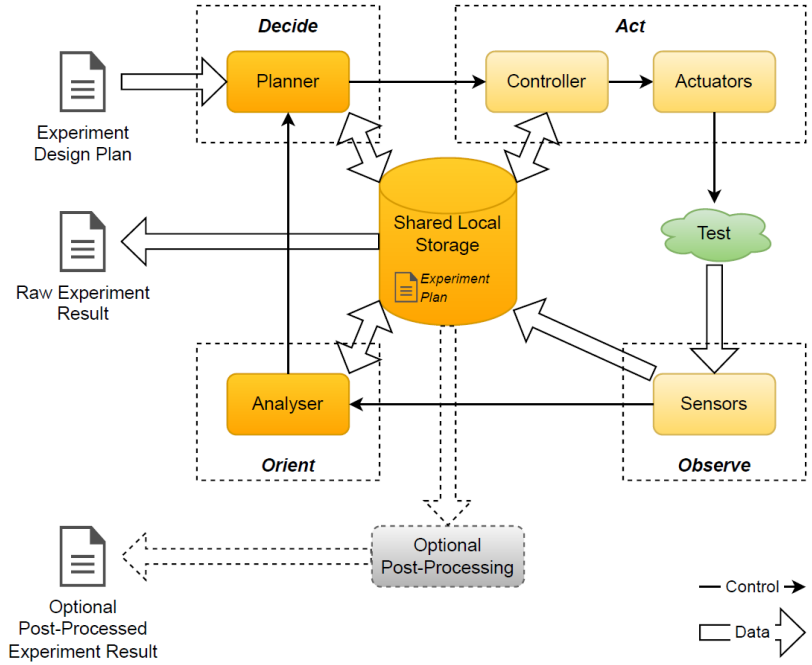


Executes existing plans (workflows of experiments)

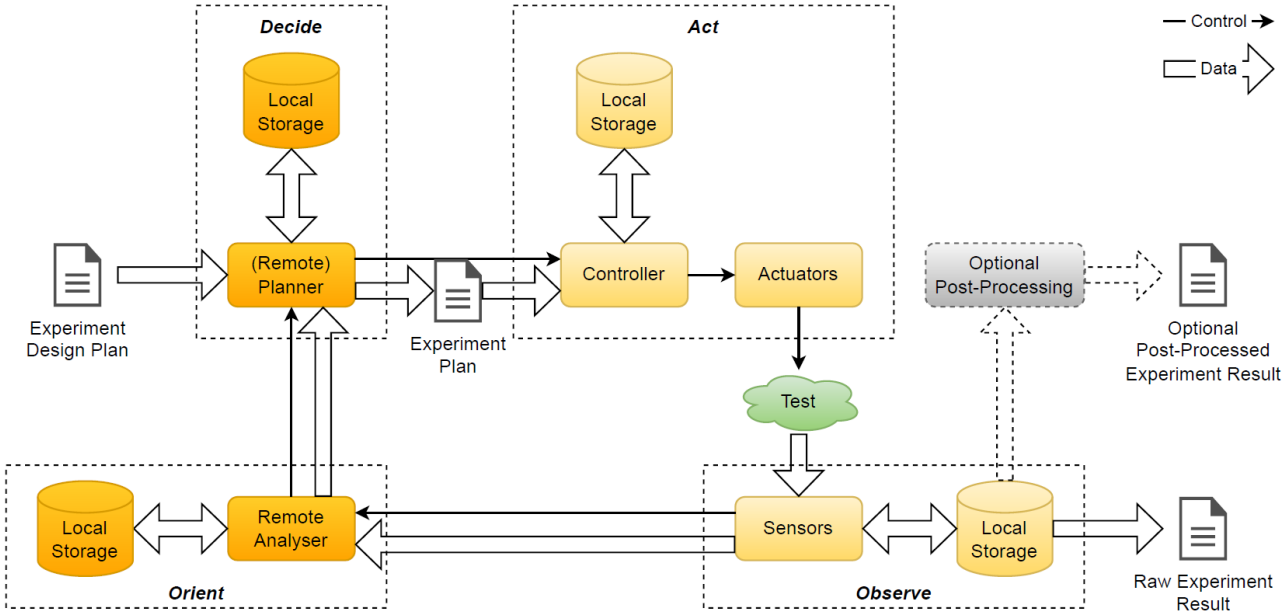
- Open loop control
- Automated operation
- User patterns:
  - Experimental Control
- May use patterns:
  - Experimental Steering
  - Design of Experiments

Nesting patterns helps ensure universality and interoperability (think Lego blocks)

Mapping Use Case Patterns on to Architectural Patterns



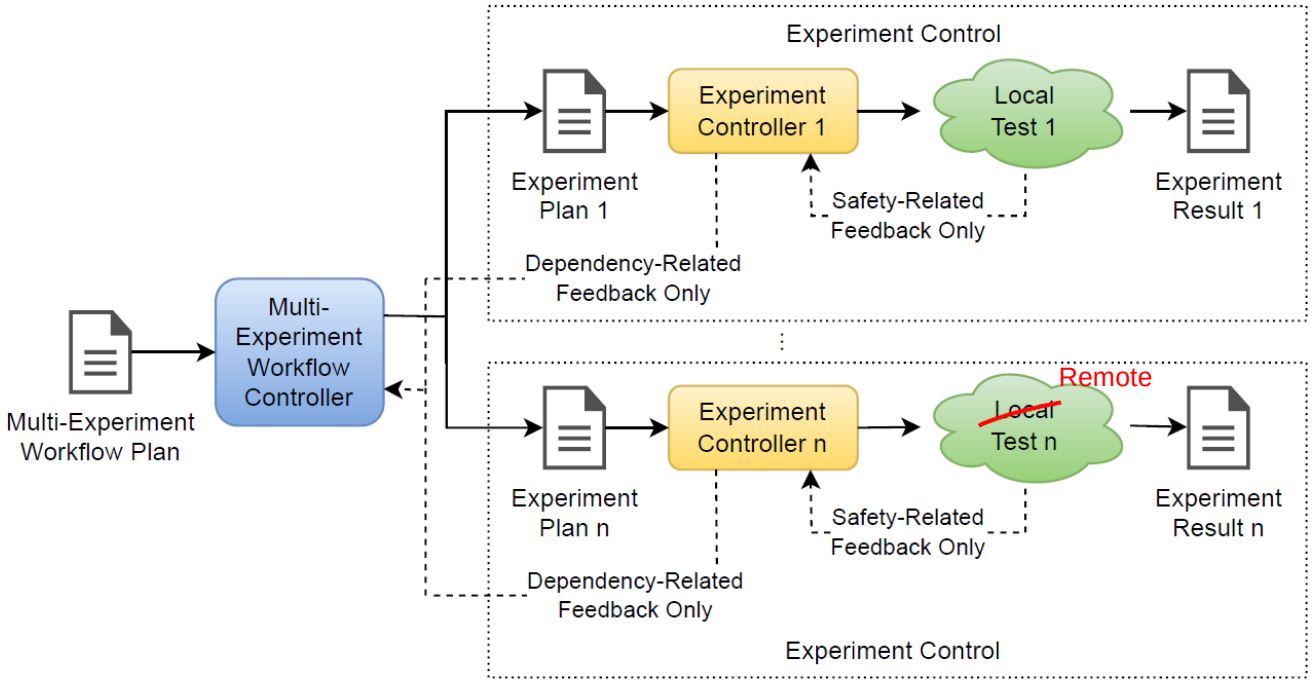
Local design of experiments

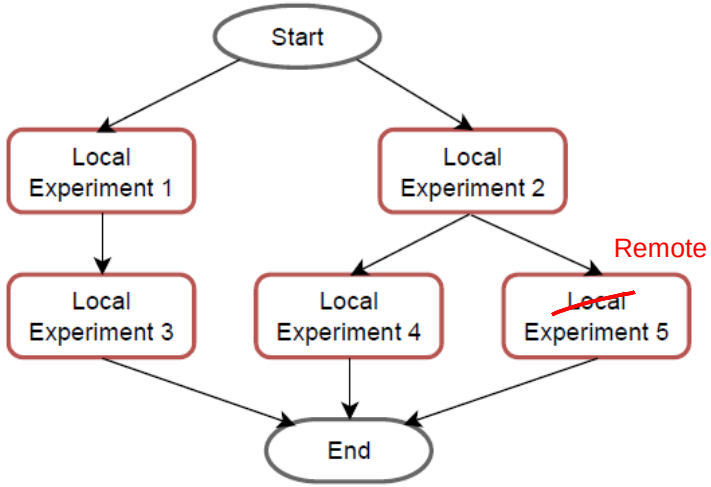


Distributed design of experiments

As with our nested strategic design patterns, we can map different strategies onto architectural patterns to understand how to move data and control experiments.

Multi-Experiment Workflows





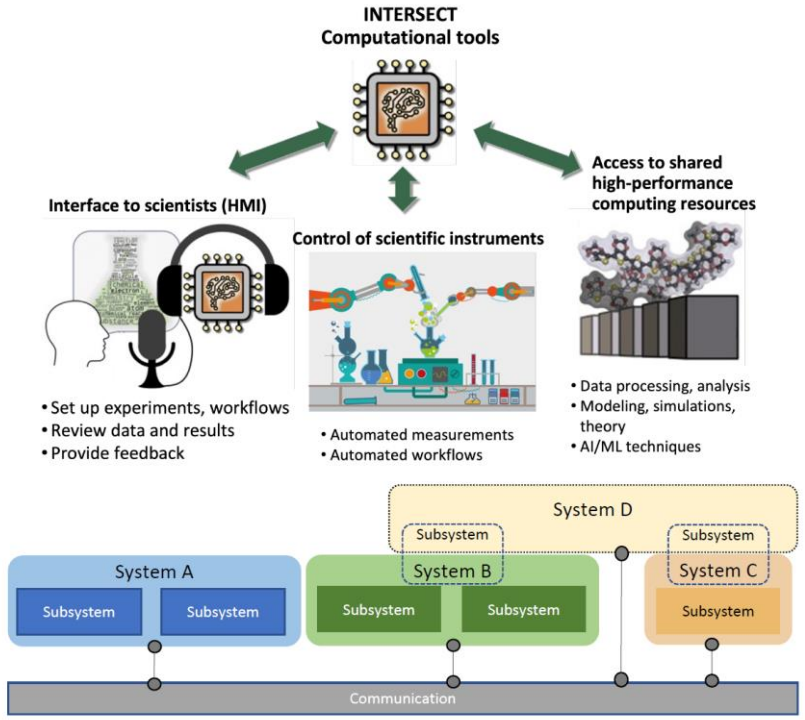
Distributed

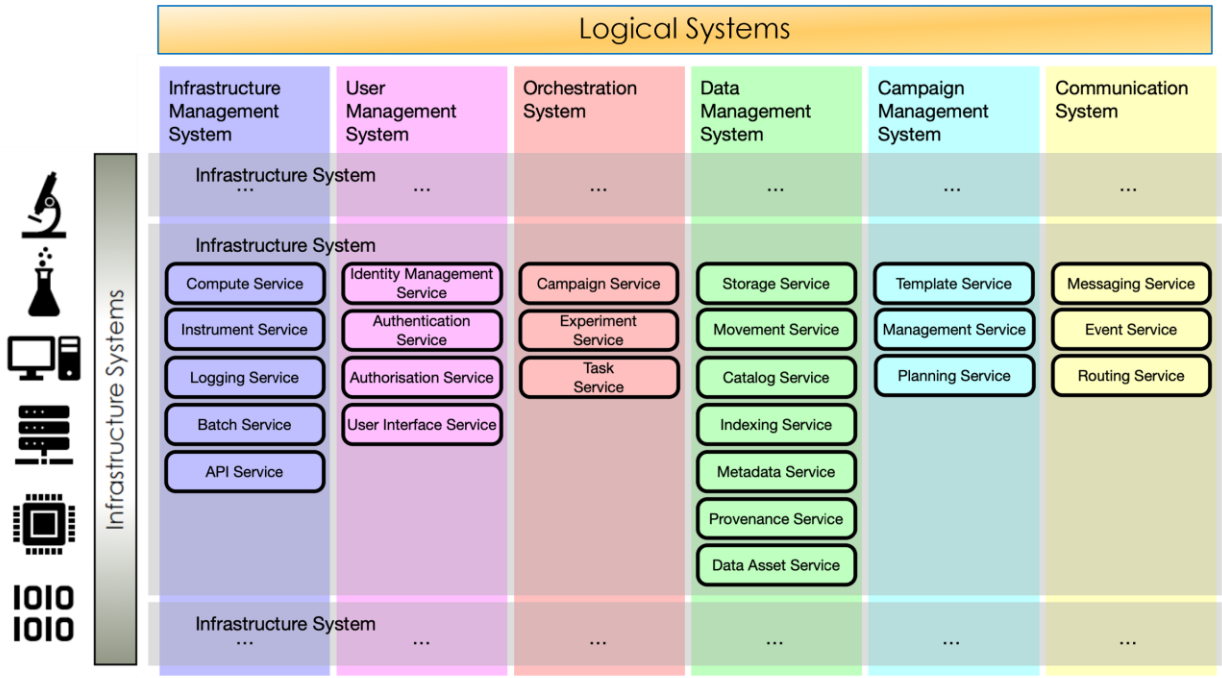
~~Local~~ multi-experiment workflow

Simplifying the connections between abstract architectural components allows for interoperability and autonomous workflows regardless of science domain or locality of resources.

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.

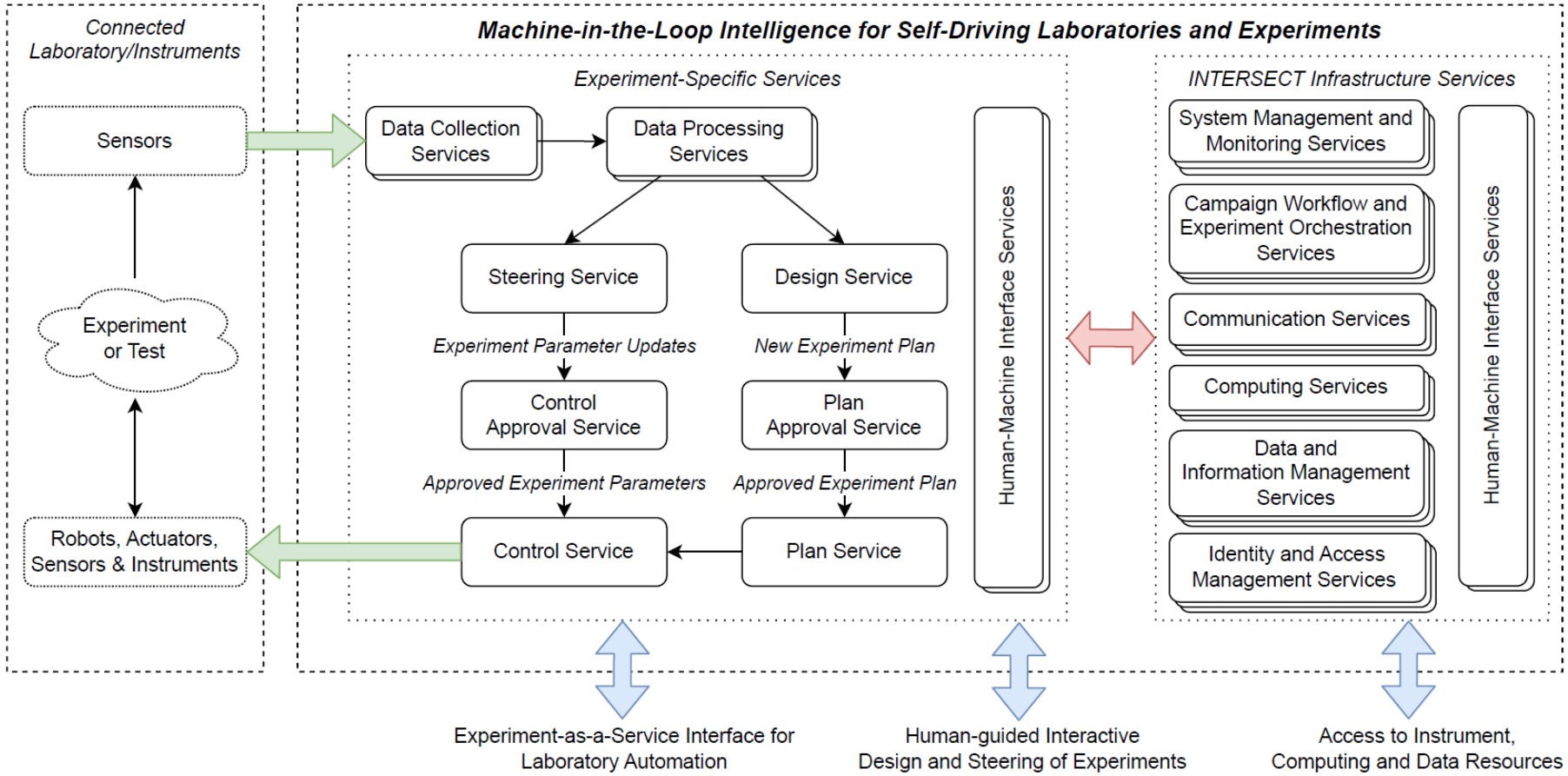




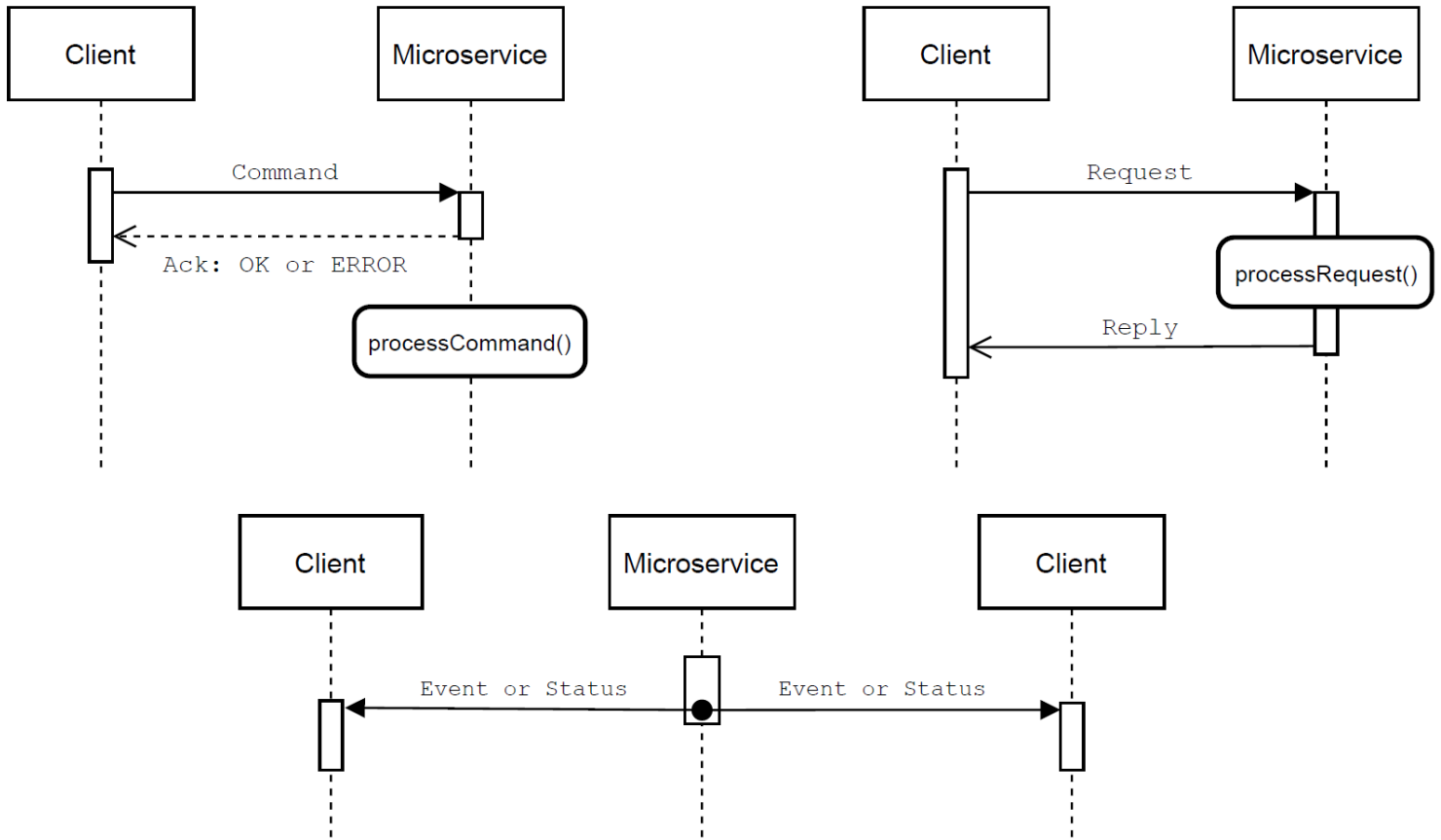
- Simple minded systems: Infrastructure Systems and Logical Systems
- Microservices provides the links which creates capabilities
- Capabilities and connections between Infrastructure and Logical systems enabled by communications via simple message passing

Microservices – From Components to Capabilities

Classes of Microservices



Communications – Connecting the Pieces



Through simple, abstract messages we can coordinate tasks and actions between architectural components using the microservices. By design, this abstract messaging layer doesn't care what resources we are coupling or where they are located.

System of Systems Ecosystem

Rapid Deployment

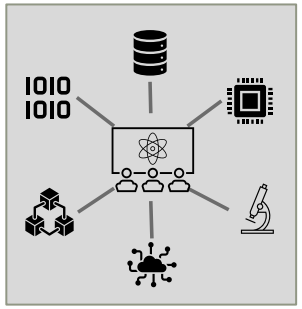
Flexibility and Reconfigurability

Interoperability

Smart Lab Marketplace

- DevOps Tools
  - Containers
  - CI/CD
- Web Portal
  - Market Webpage
  - ...

Autonomous Labs



Ecosystem Software Services

- Exposing Resources
  - System Adapter
  - Subsystem Adapter
- Orchestration
  - Workflow Manager
  - Approval Manager
- Autonomy / Automation
  - Contingency Manager
  - Autonomy
- Cybersecurity
  - Authent. / Author.
  - Cyber Monitor
- Human Machine Interface
  - Web Portal
- Data Management
  - Storage
  - Movement
- Data Analysis/Computation
  - AI Analysis
  - Simulation
- Other
  - ...
  - ...

Abstraction Layers

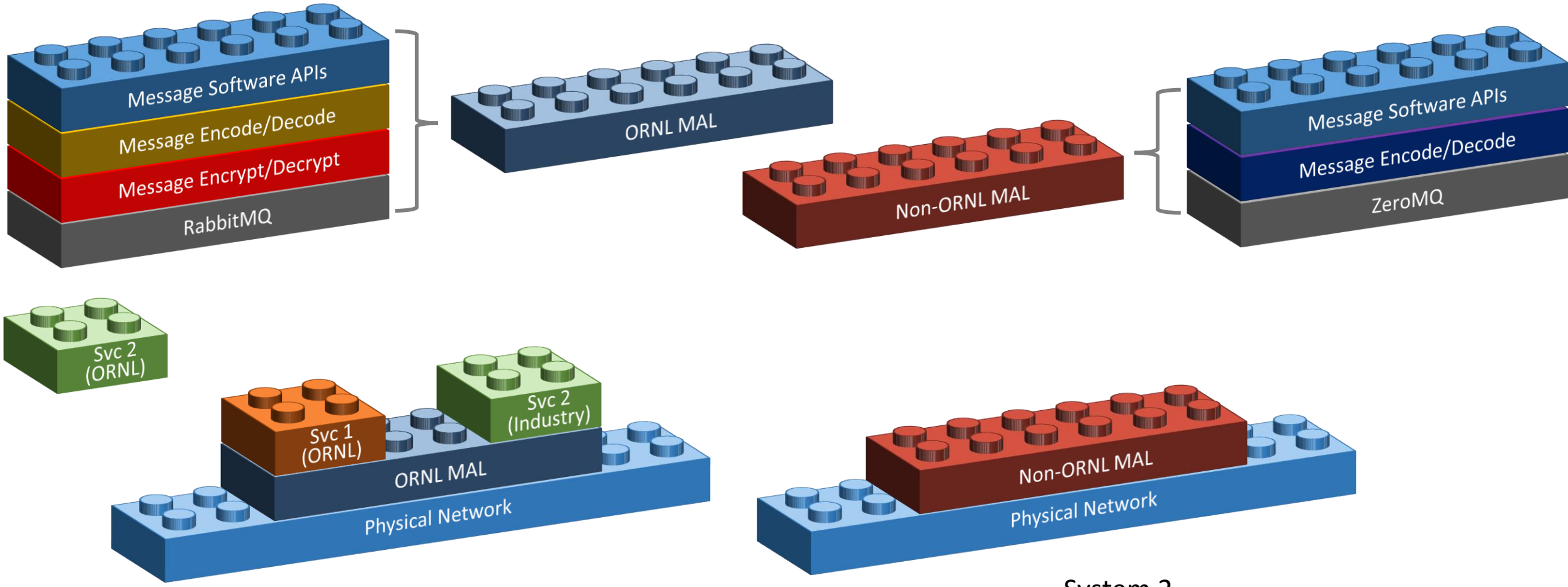
- Control Plane
  - Message Abstraction Layer
  - MQTT
  - RestAPIs
  - ...
- Data Plane
  - Scientific Data Layer
  - Globus
  - Stream Data
  - ...

Physical Infrastructure

- Instruments
- Compute
- Databases
- Equipment
- Facilities
- ...

Why Develop an Abstraction Layer

- Flexible software reuse through the common/open Message Software APIs
- Avoid vendor-lock to enable contributions from multiple teams (e.g. DOE, Industry, and Academia)
- Enable plug-and-play integration testing to find the best-of-breed software



System 1

System 2

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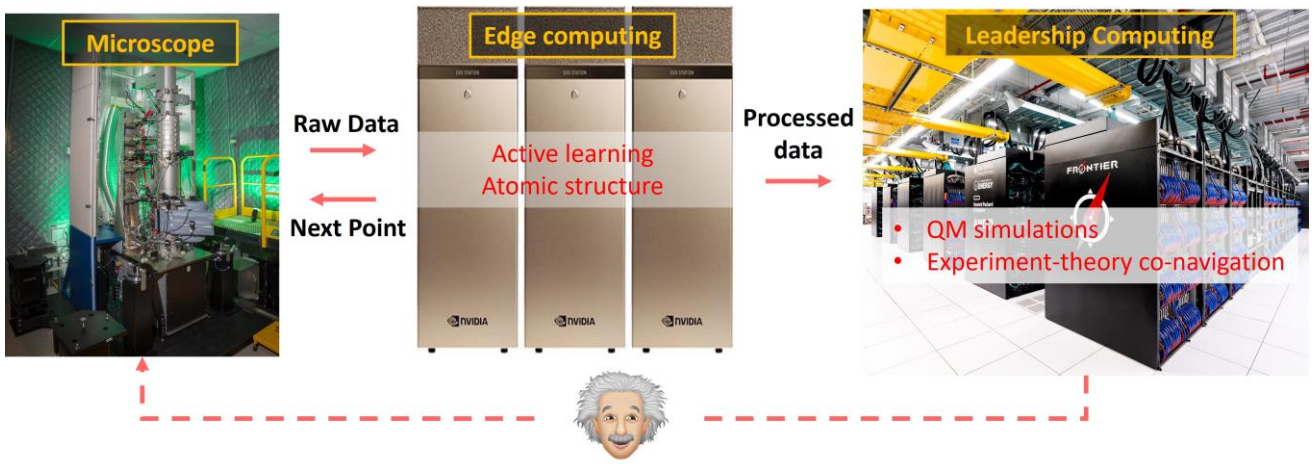
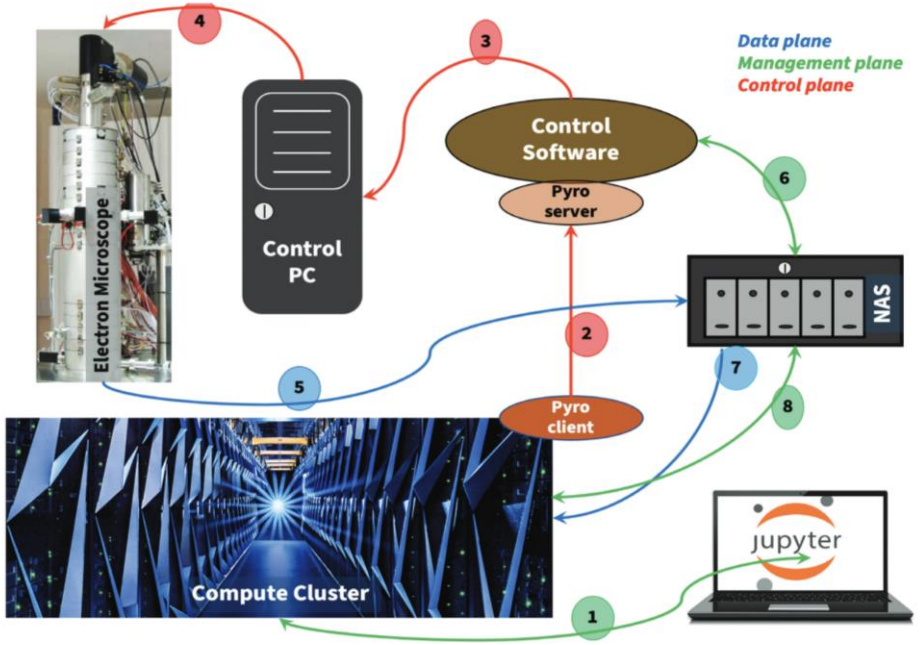
Use Cases

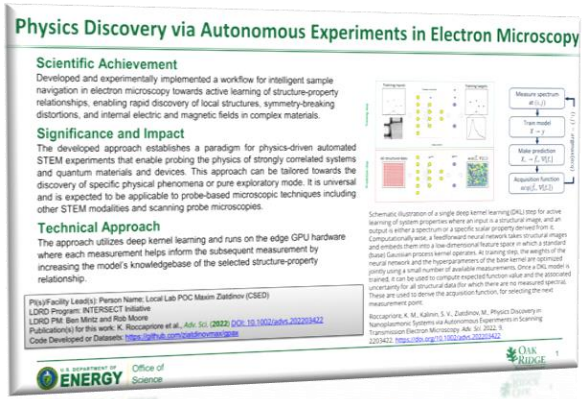
Autonomous Scanning Transmission Electron Microscope

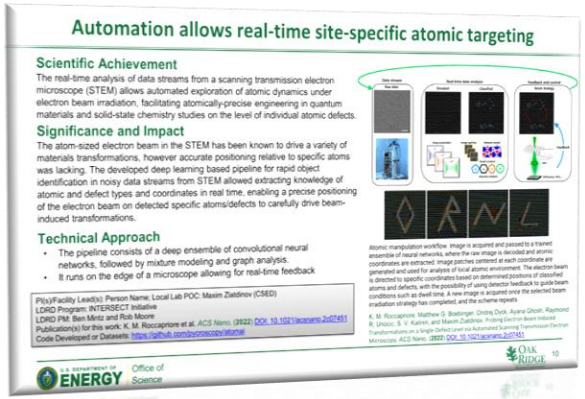
Autonomous Experiments in Electron Microscopy





- **Limiting steps:** data, computation, control
  - Data: large volumes (Can generate 1TB in ~15 min)
  - Computation: analysis on the fly via deep learning, feed into theoretical models
  - Control: real time feedback to choose the places for study and control beam changes towards desired discovery and fabrication outcomes





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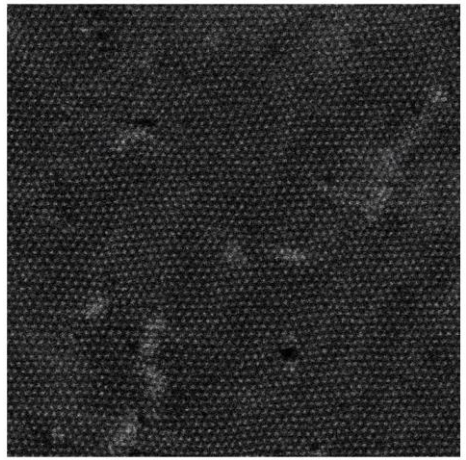
Autonomous Experiments in Electron Microscopy

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

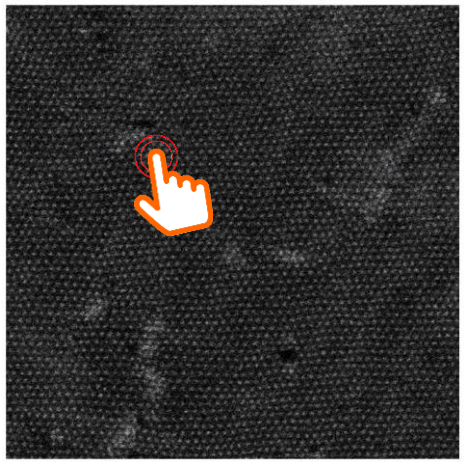
Microscope

Raw data



Human scientist

Features of interest

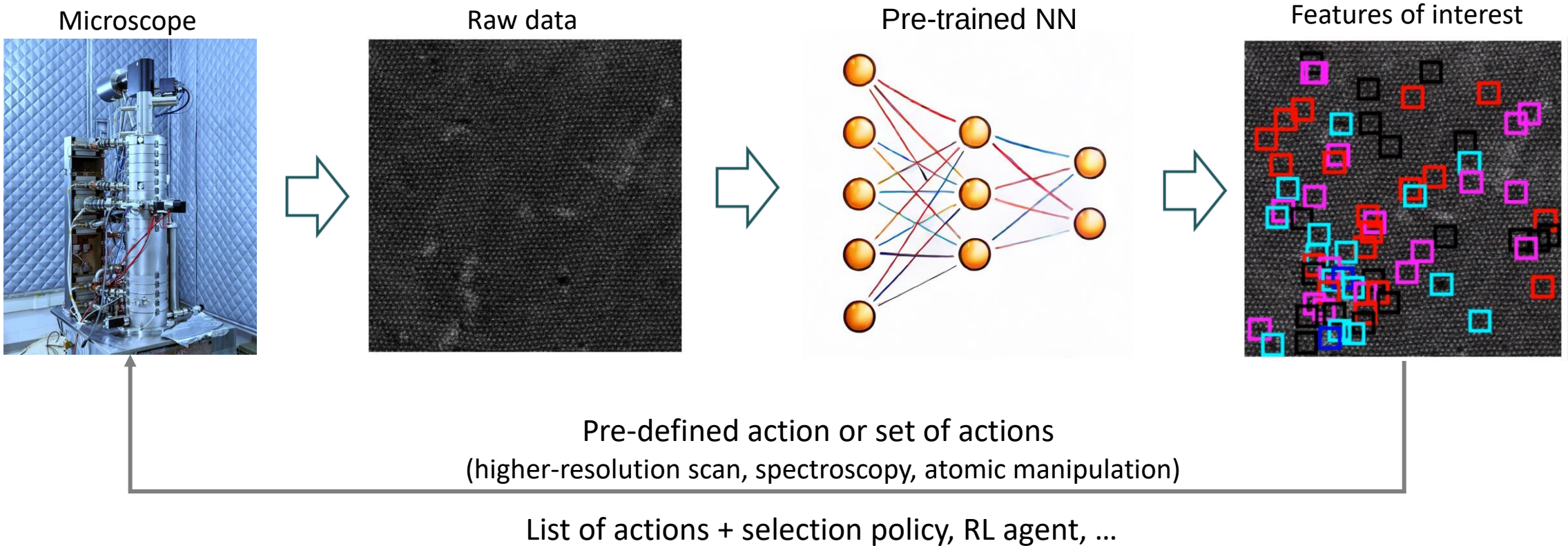


Pre-defined action

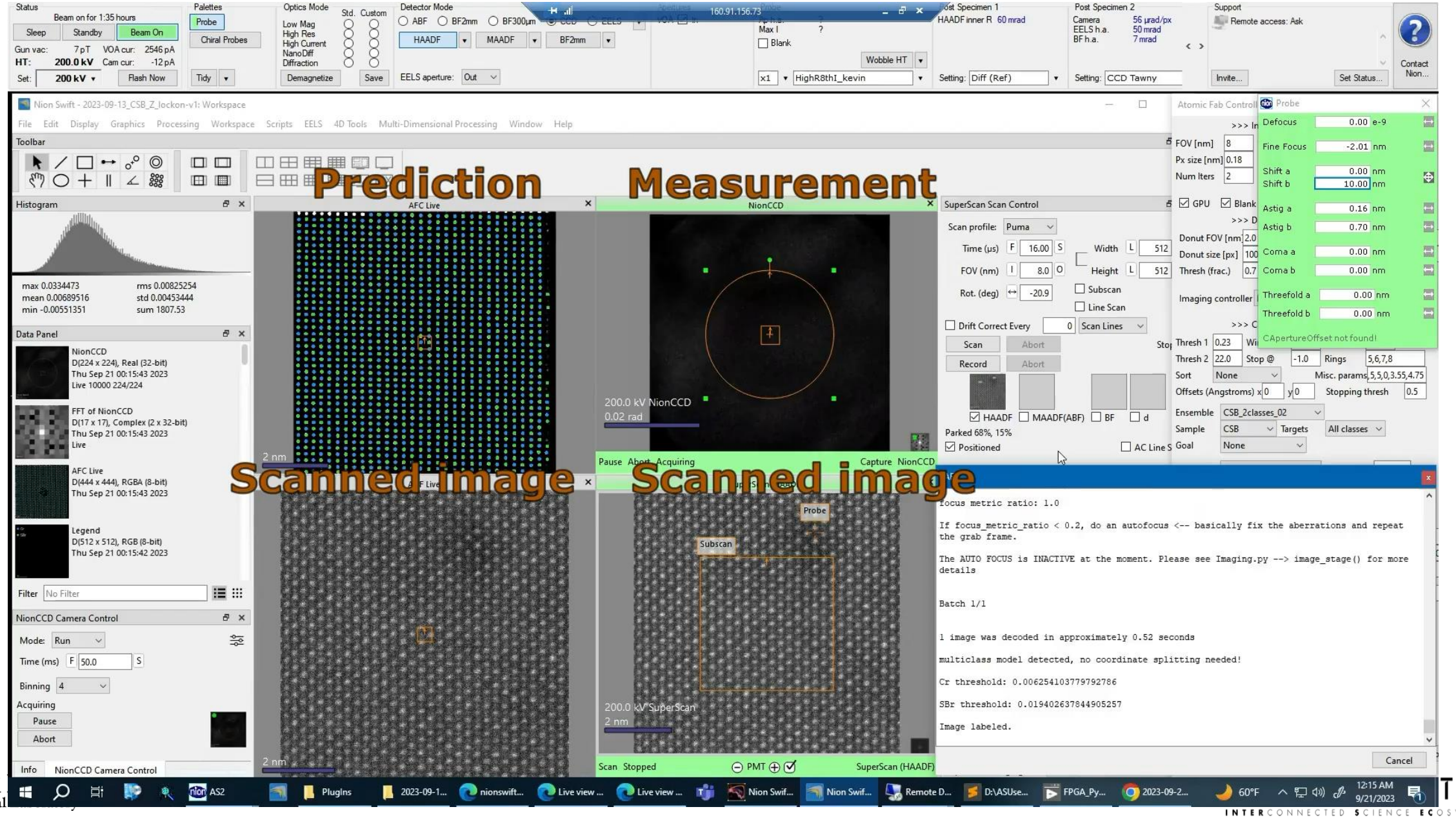
(higher-resolution scan, spectroscopy, atomic manipulation)

Autonomous Experiments in Electron Microscopy

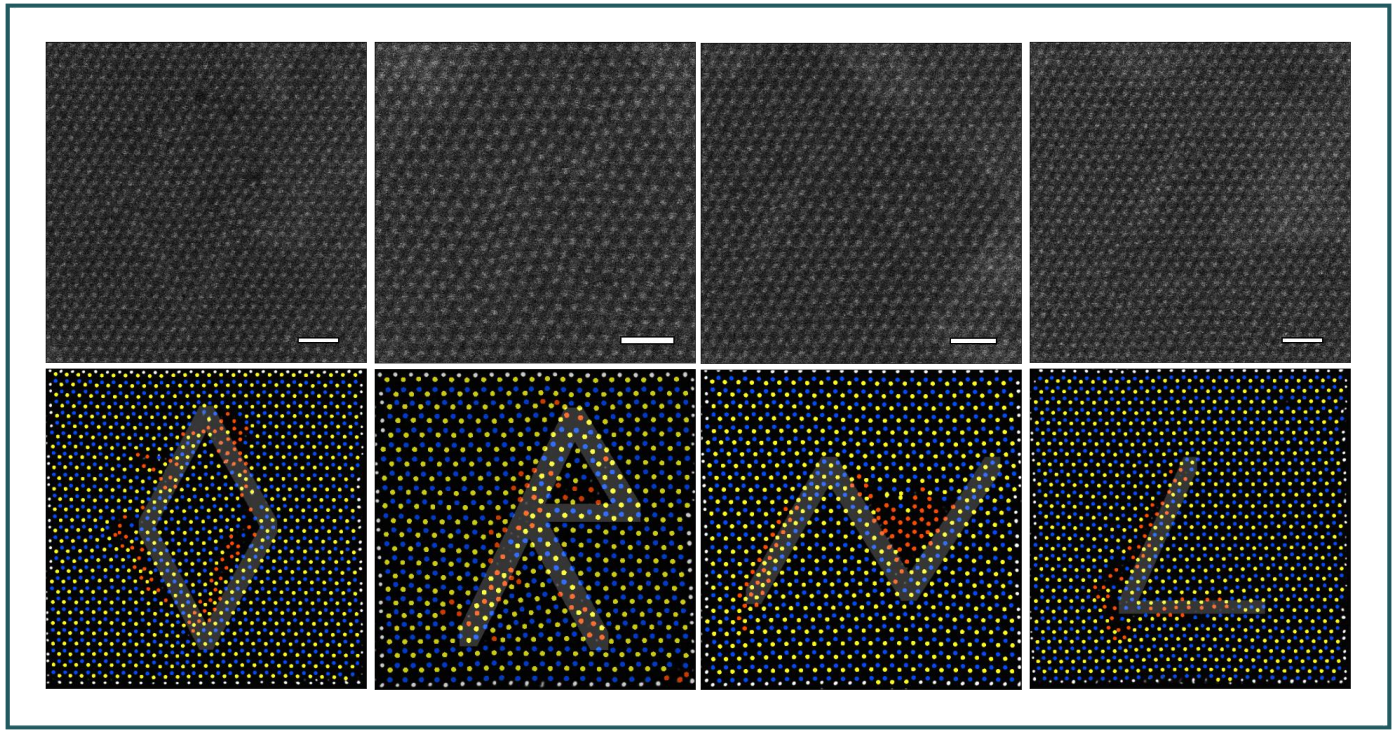
Rapid object detection and action system (RODAS) - *a priori* defined objects of interest that can be recognized in real time with a pre-trained neural network.



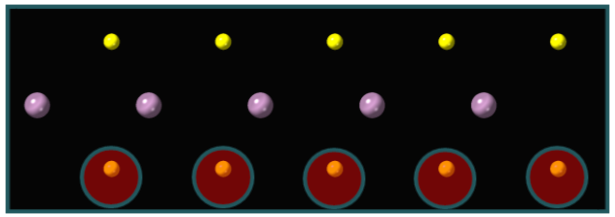
Rapid object detection and action system - DEMO

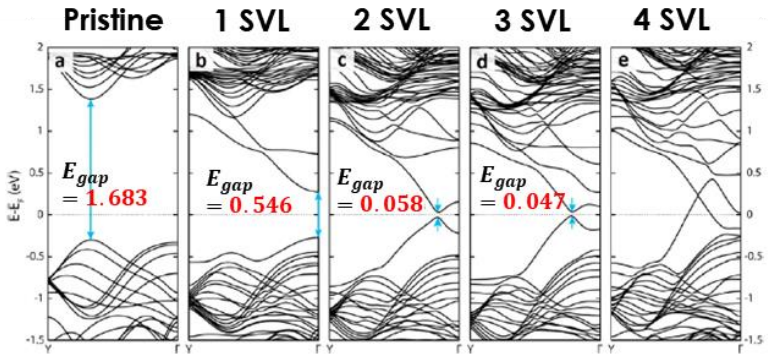


Next Step: From Structure to Property to Control

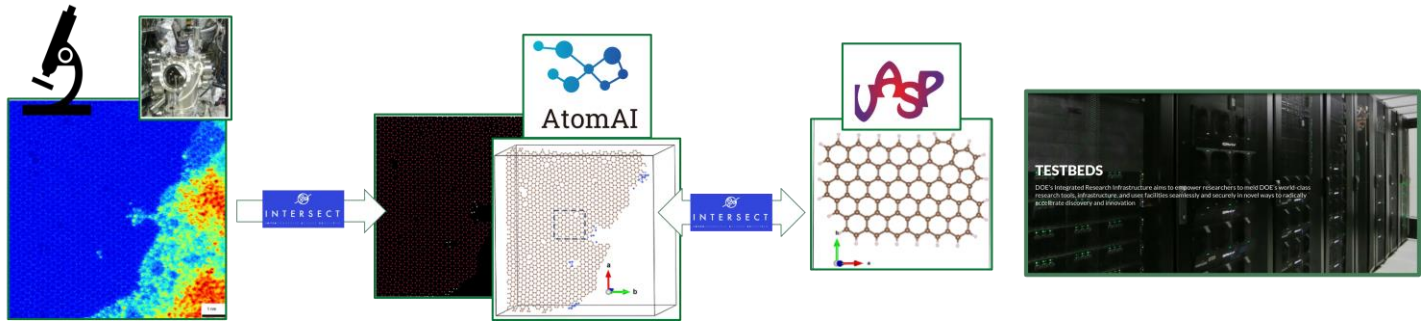


MoS_2





Instrument Edge HPC



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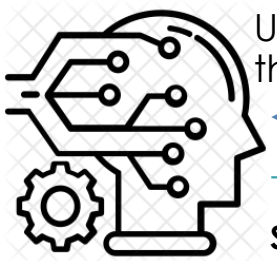
INTERSECT
INTERCONNECTED SCIENCE ECOSYSTEM

Autonomous Continuous Flow Reactor Synthesis

Autonomous Continuous Flow Reactor Synthesis

- Periodic system status information
- Experimental status information triggered throughout the experiment

Step 5: System 4 completes the experiment; feedback is autonomous



User views status of the various systems

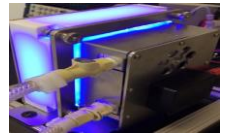
System 1
(includes HMI)

I-API

System 2

Continuous flow reactor

INTERSECT to EPICS translation



System 4
(Running EPICS)

Step 1: User creates the experimental plan using system 1
a) runs system 2
b) sends data to system 3 for analysis
c) starts system 4 with input from edge analysis

Step 2: User begins the experiment plan; setting which modes of in-line characterization will be used

Step 3: System 2 runs the first part of the experiment and data acquisition

Step 3.5: Data streams queued from System 2 are transferred to System 3

System 3

Edge Analysis Node(s)

Step 4: Edge analysis of the data

Step 4.5: Data transfers from System 3 to System 4

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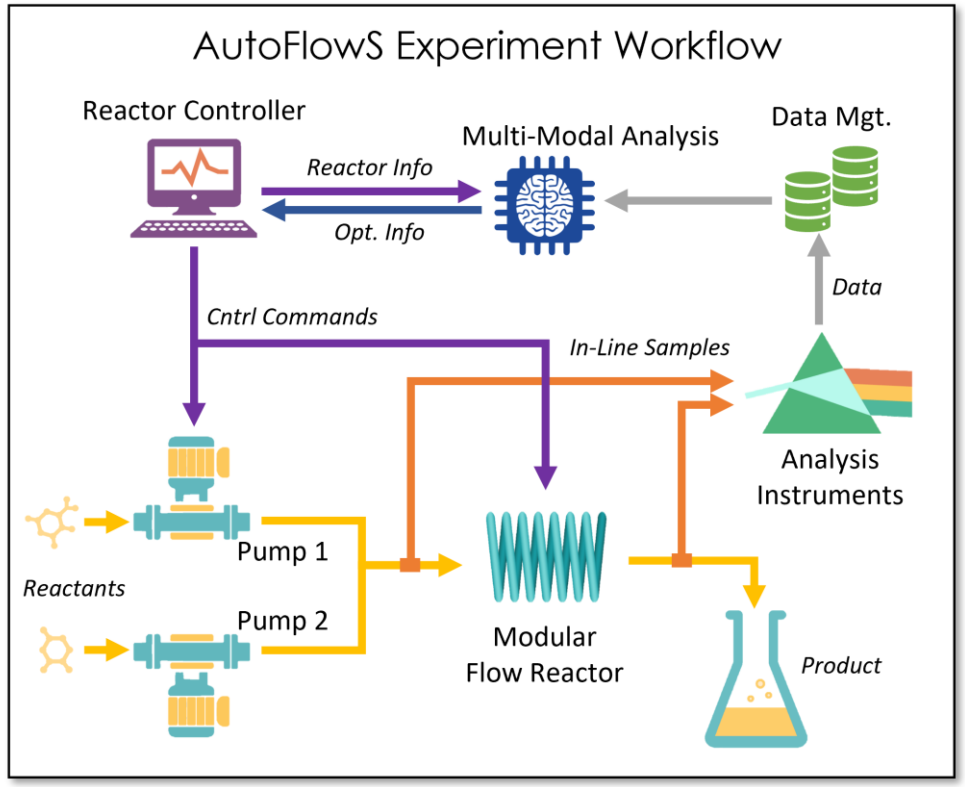
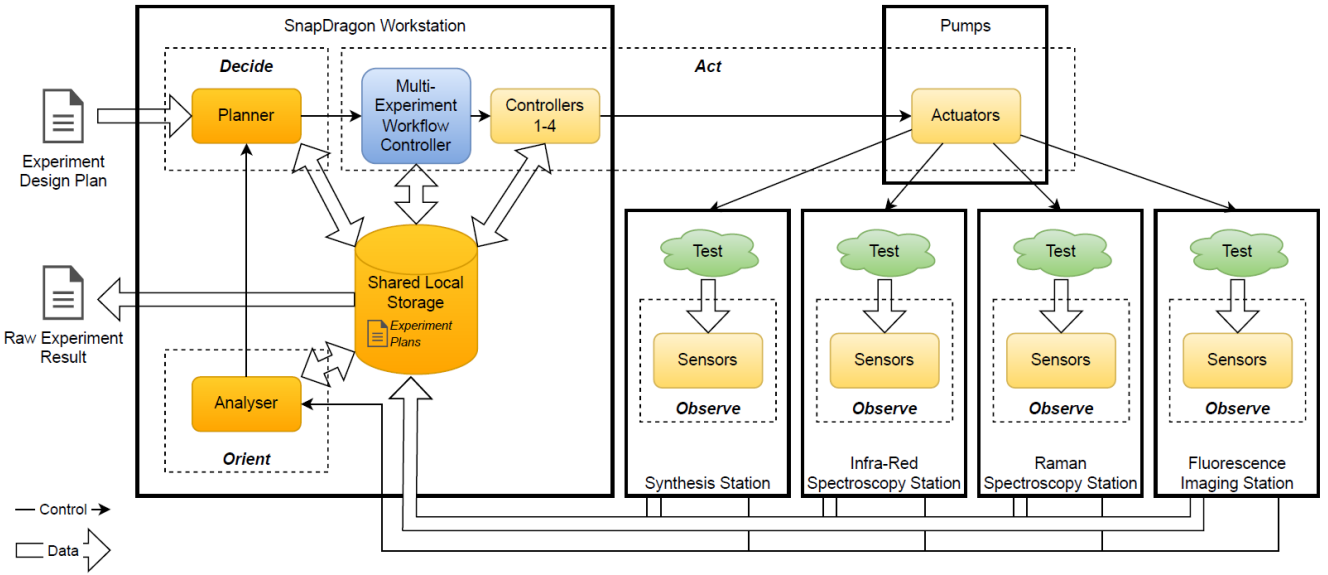
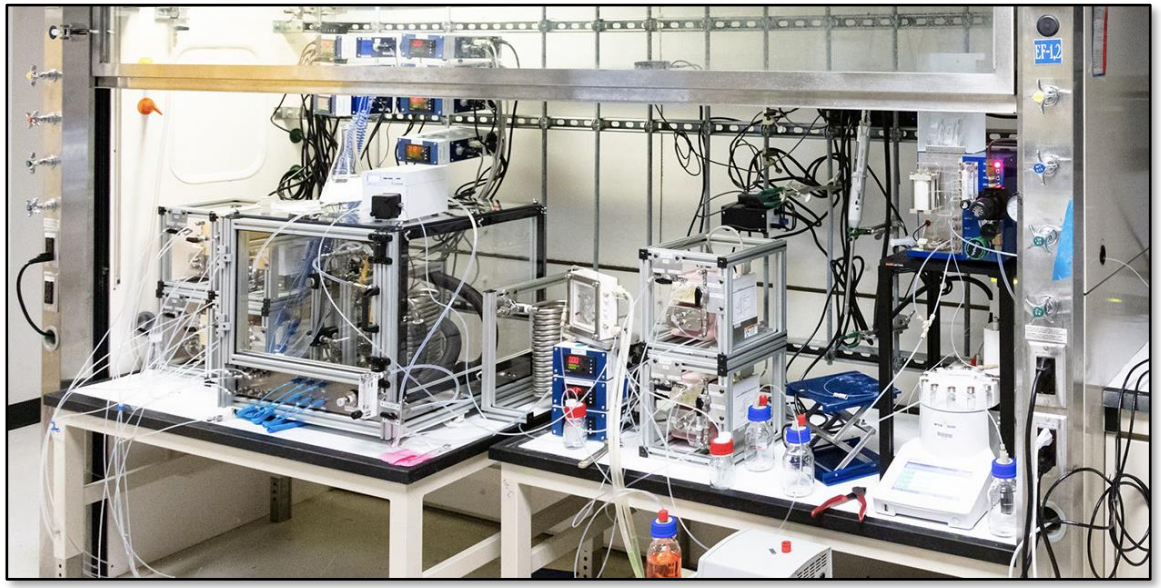
INTERSECT
INTERCONNECTED SCIENCE ECOSYSTEM

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

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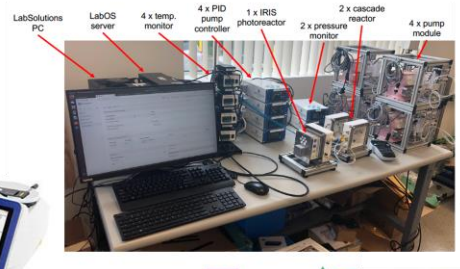
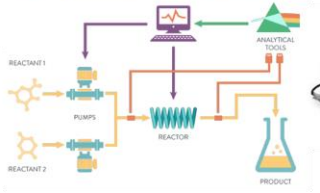
INTERSECT
INTERCONNECTED SCIENCE ECOSYSTEM

Autonomous Workflows in Action

Current Suite of Instruments



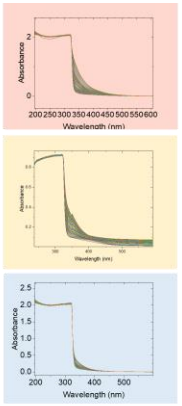
IR/Raman
NMR
ESR
RI
SPR
UV/Vis
Fluorescence
Electrochemical
QCM
Viscosity



Auxiliary Flow Reactor (ThalesNano Syrris, Vapourtec): Instrument/Sensor Interfacing

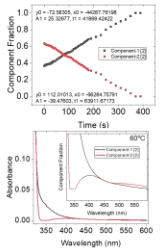
Multi-modal Workflows

NMR
FTIR
Raman
GPC
Scattering
QCM



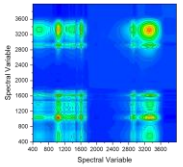
T-dependent homopolymerization

Thermodynamics
Rate constant
Product signatures



PCA, MCR

Correlation spectroscopy homo/hetero



Unique signature of material → Large scale synthesis for 3D

Predictive modeling of process dynamics and thermodynamics

ML in Action

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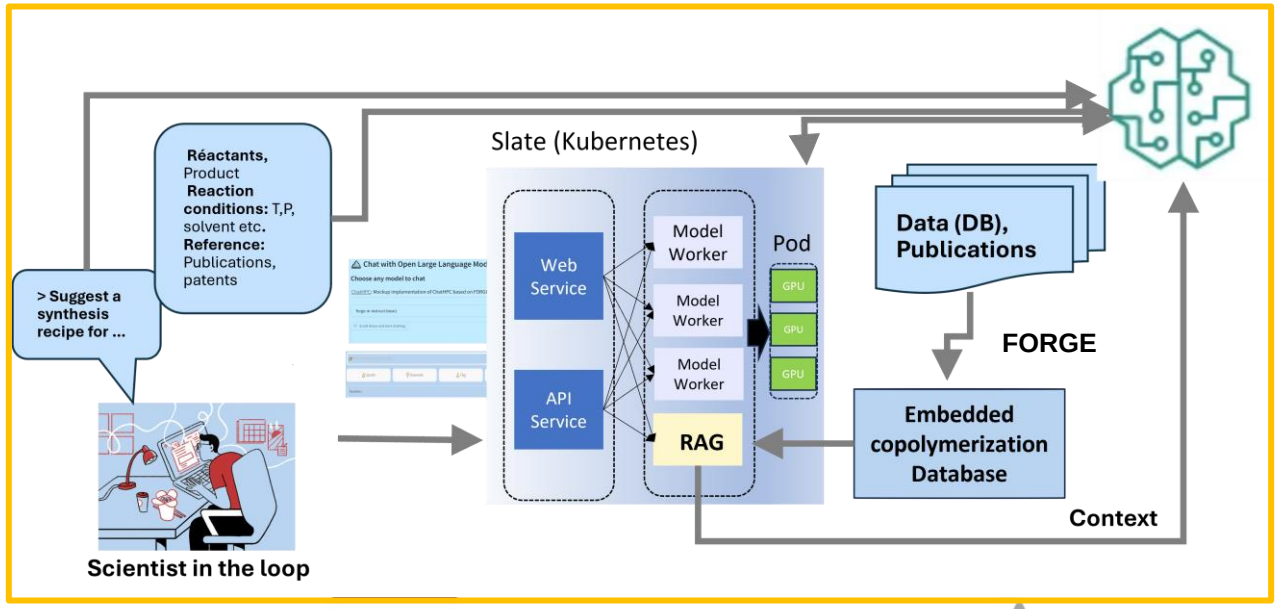
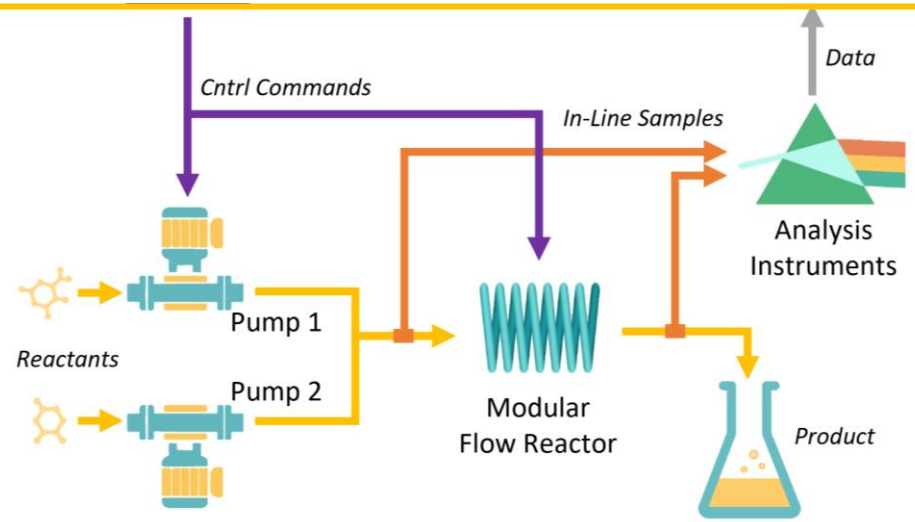
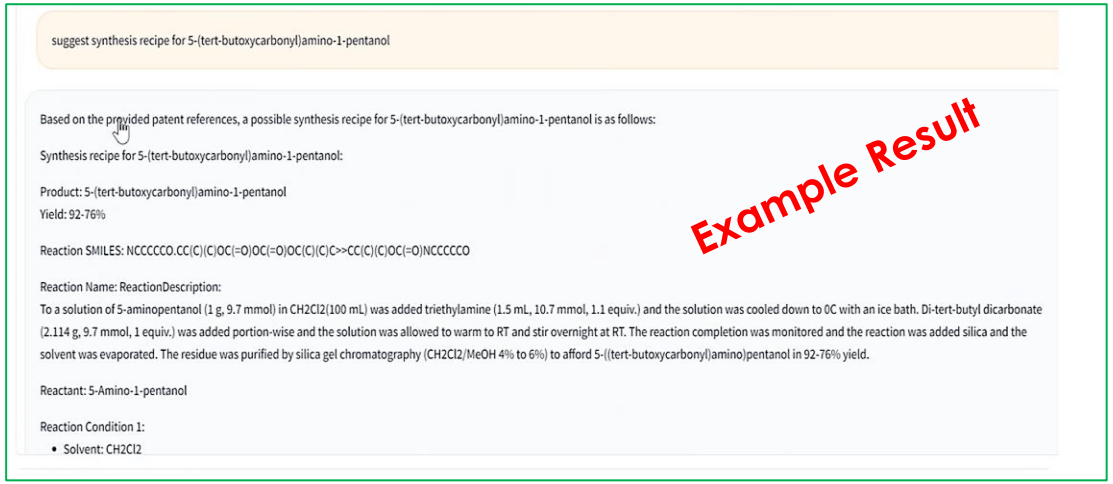
INTERCONNECTED SCIENCE ECOSYSTEM

AutoFlowS + 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







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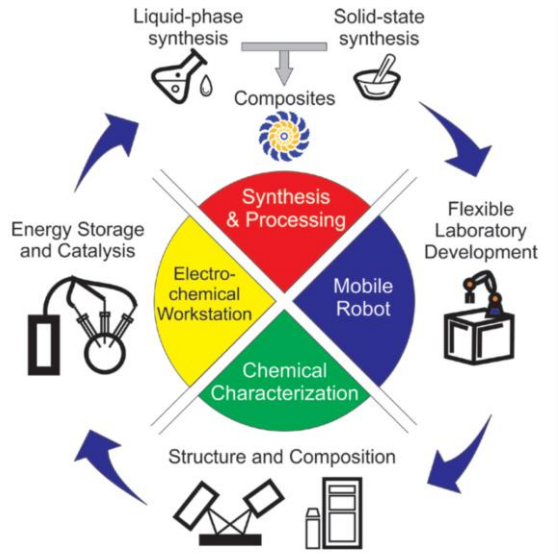
CNMS OLCF

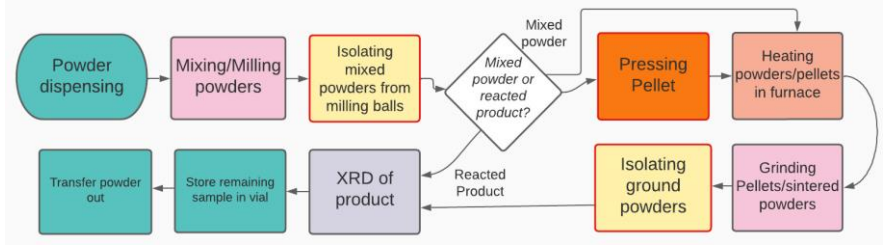
INTERSECT
INTERCONNECTED SCIENCE ECOSYSTEM

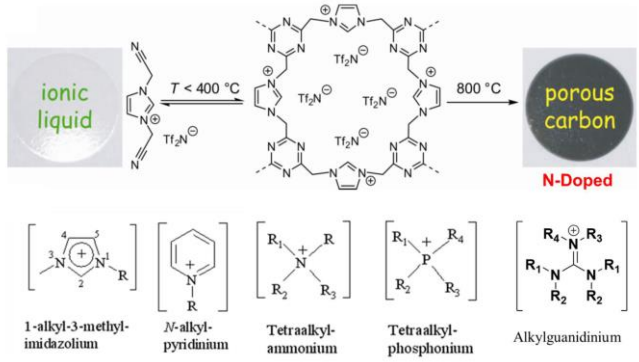
Autonomous Chemistry Laboratory

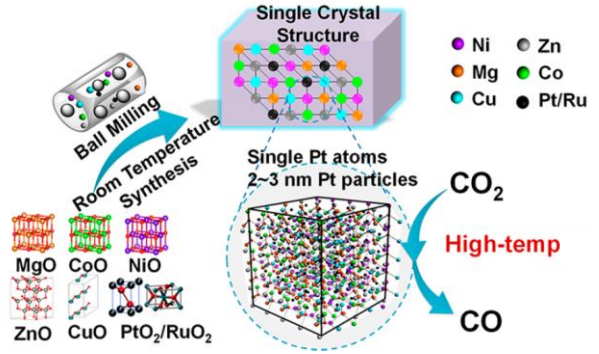
Autonomous Chemistry Laboratory (ACL)



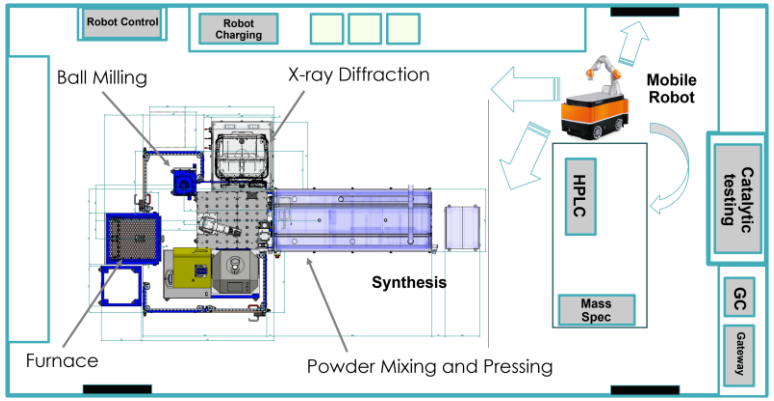
Autonomous Materials Workflows for Catalysts

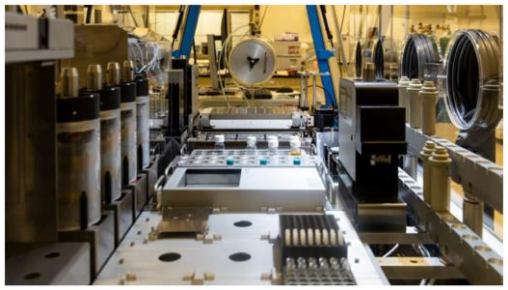


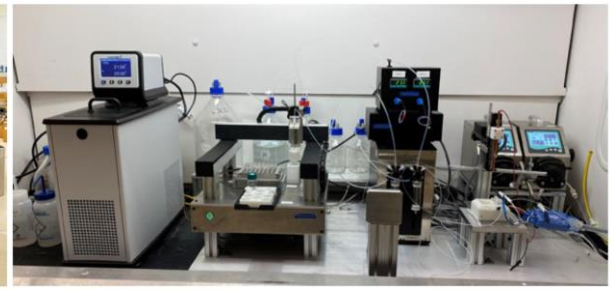




Robotics Chemistry Laboratory







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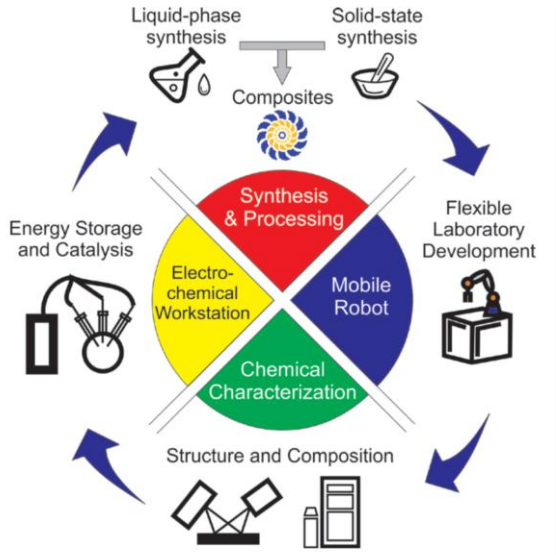
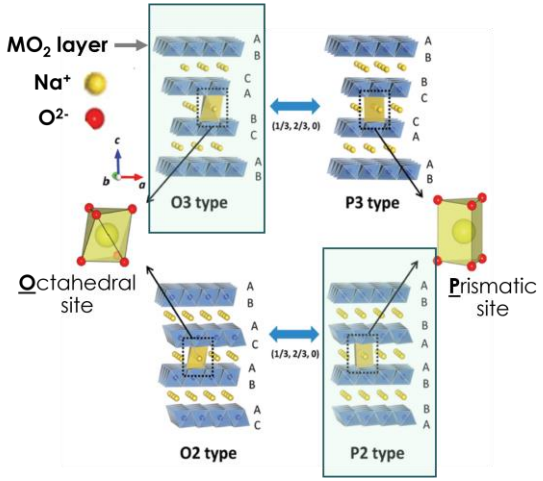
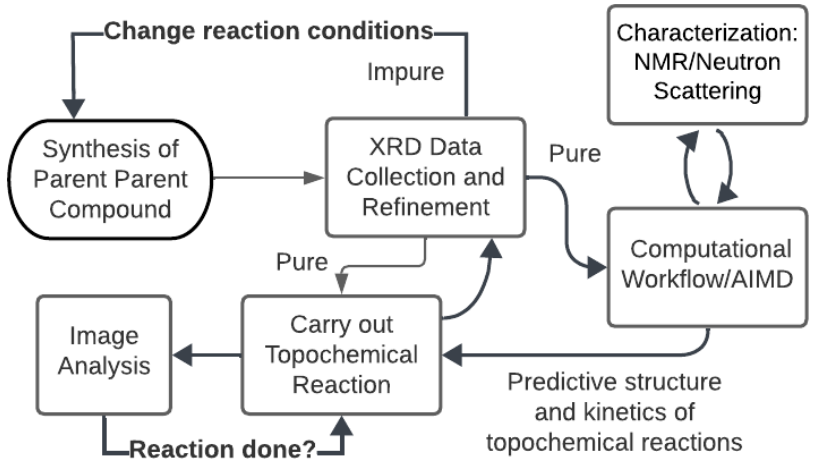
INTERSECT
INTERCONNECTED SCIENCE ECOSYSTEM

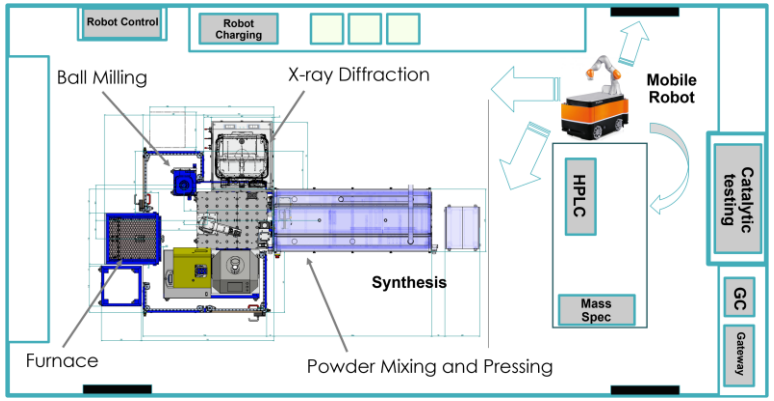
Autonomous Chemistry Laboratory (ACL)



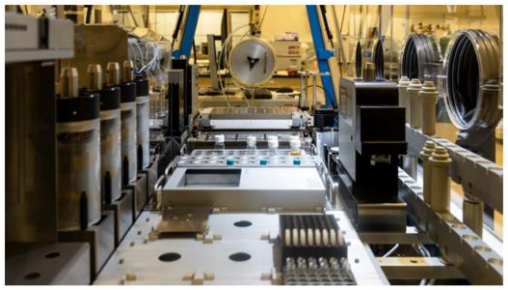
Autonomous Topochemical Synthesis Workflows for Na-ion Battery Cathodes

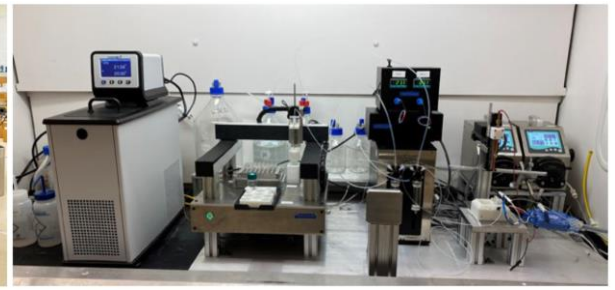






Robotics Chemistry Laboratory





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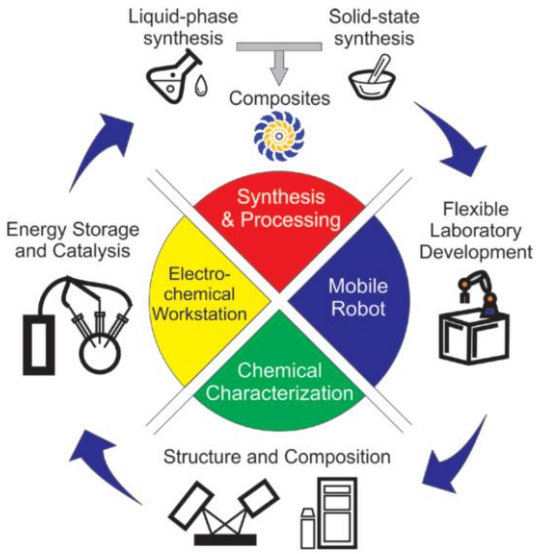
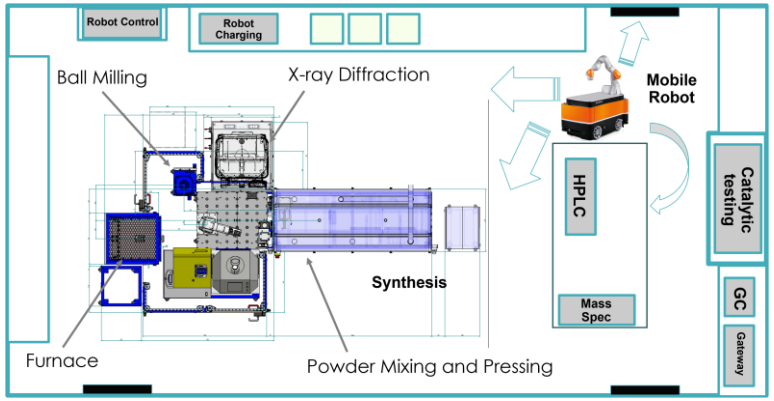
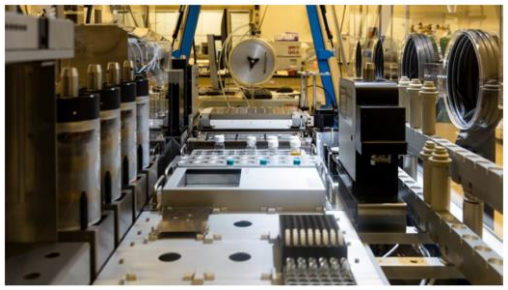
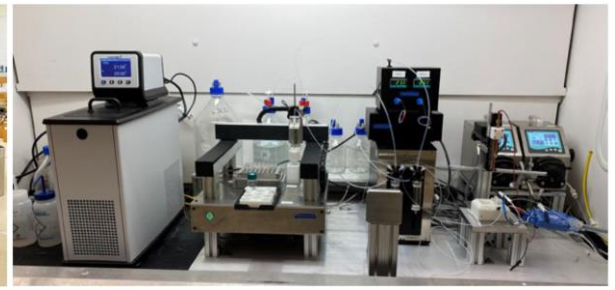
Autonomous Chemistry Laboratory (ACL)





Robotics Chemistry Laboratory





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Autonomous Additive Manufacturing

Additive Manufacturing – 3D Printing of Anything

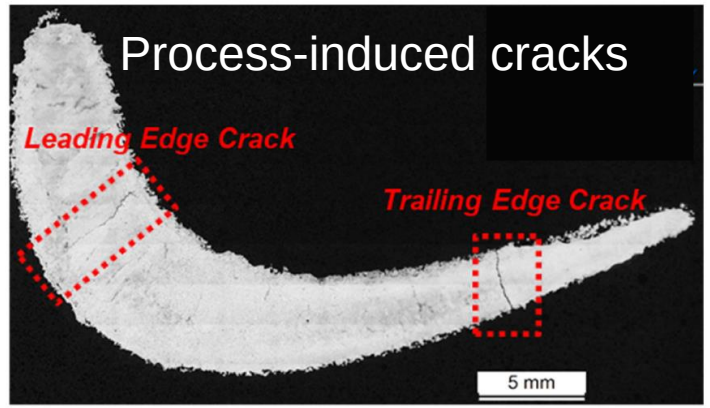
AM: Building a part layer-by-layer by melting small amounts of powder/wire at a time

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



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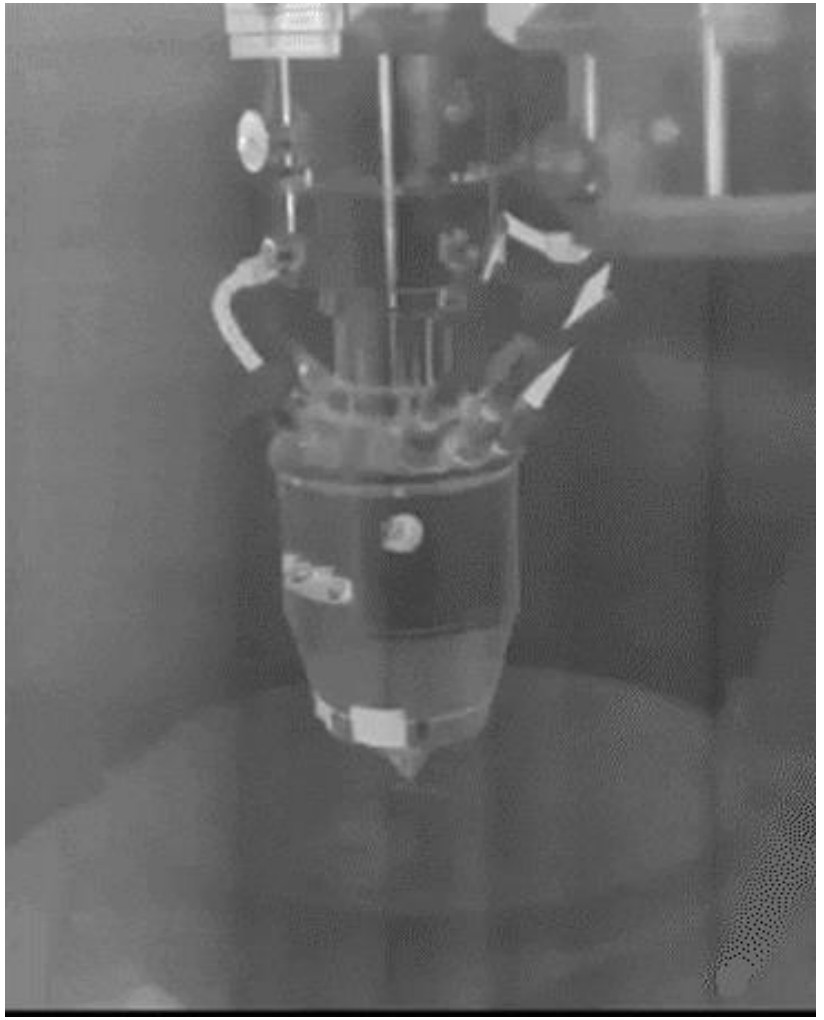
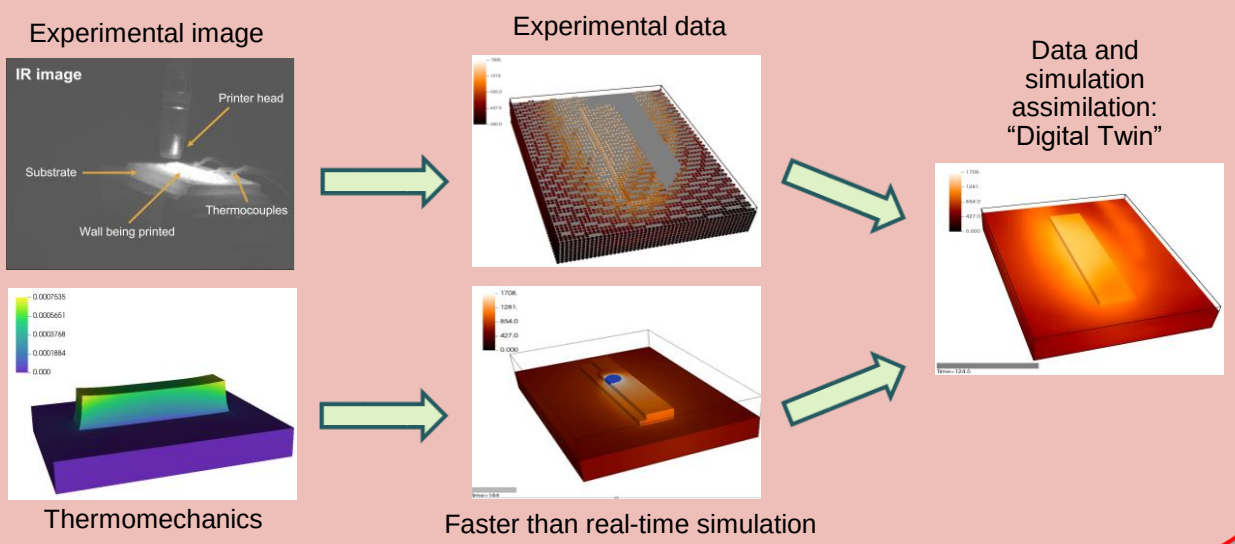


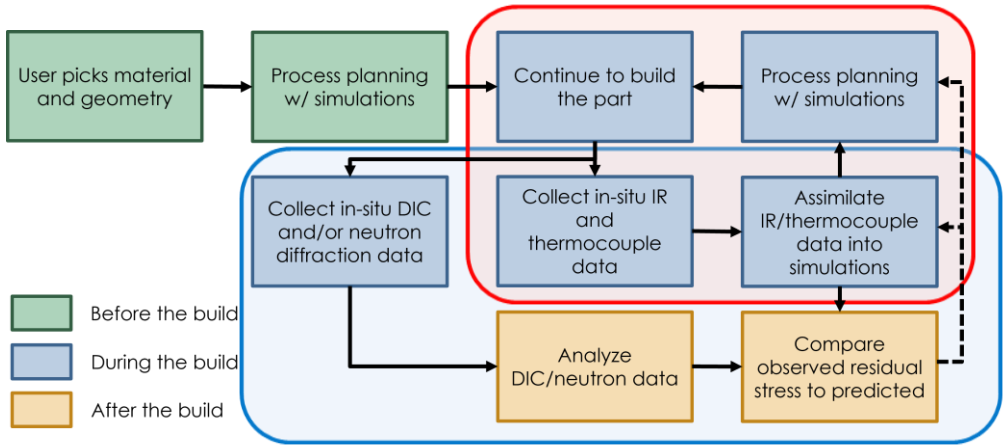
Lee, et al, Additive Manufacturing, 2020.

Autonomous Additive Manufacturing

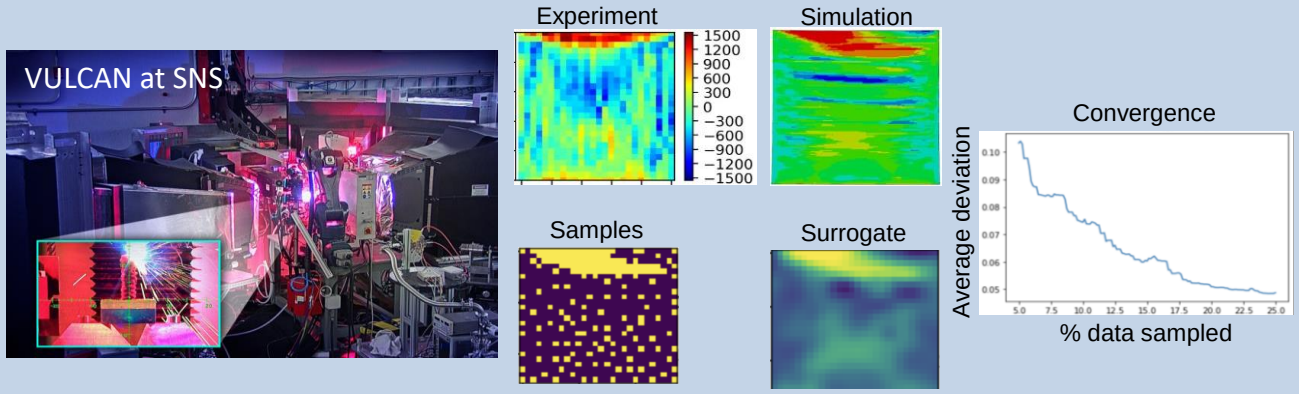
Additive Manufacturing Digital Twin



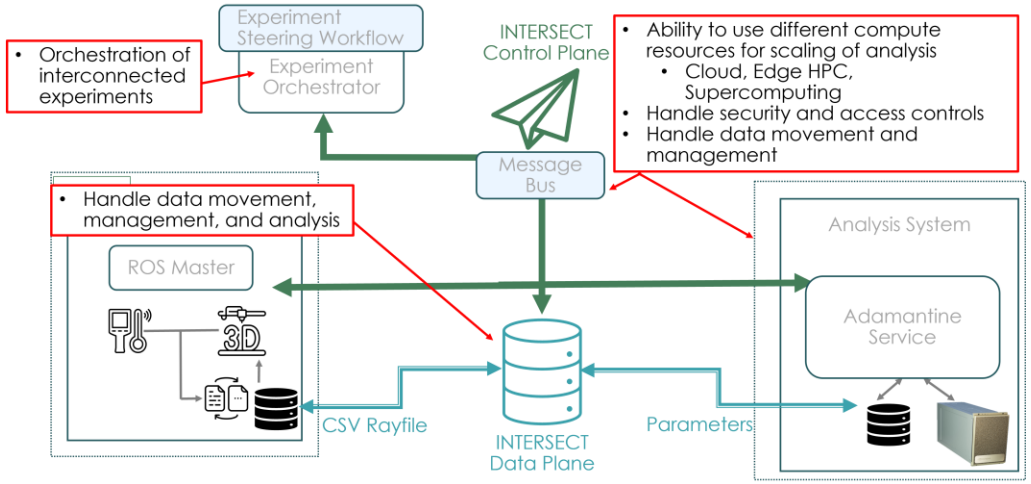
Additive Manufacturing Autonomous Workflow



Additive Manufacturing / SNS Integration



INTERSECT Software Services



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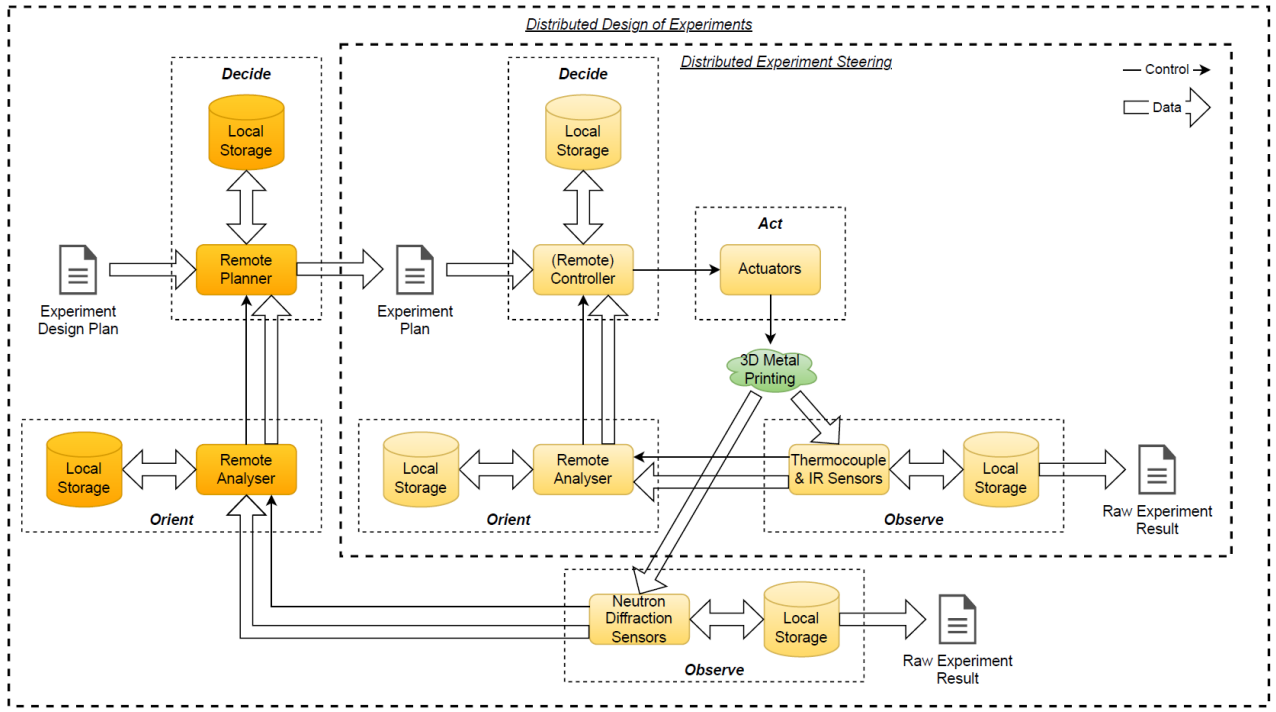
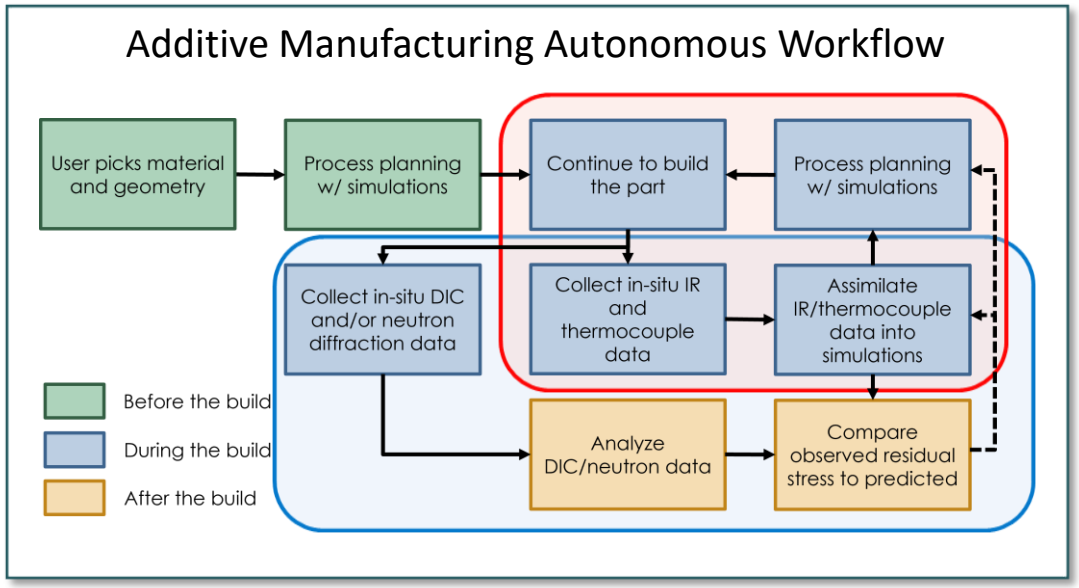
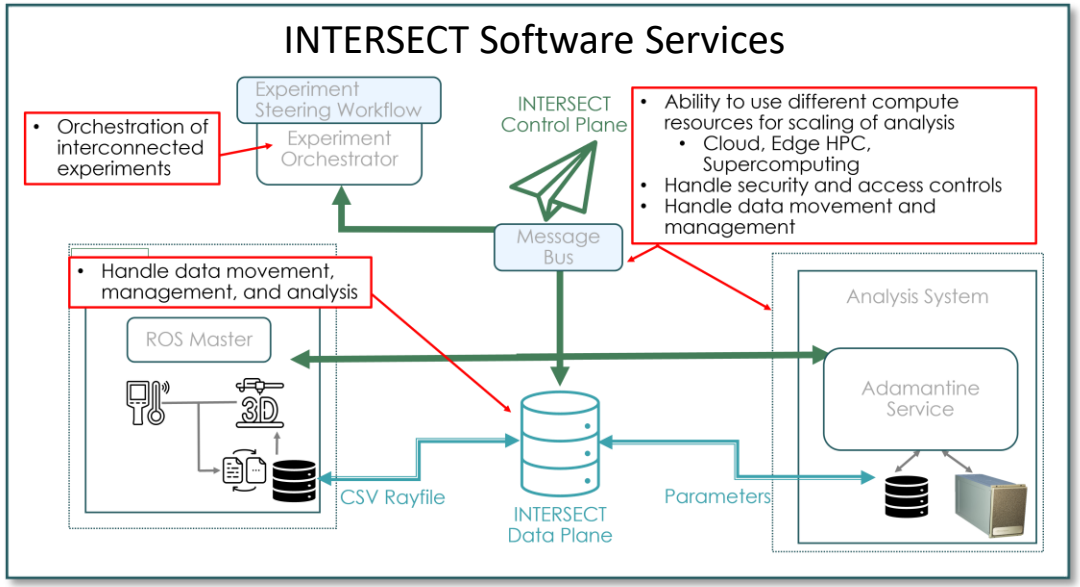
INTERSECT INTERCONNECTED SCIENCE ECOSYSTEM

Autonomous Additive Manufacturing



- Interconnected workflows – IR Sensors and Neutron Diffraction
- Mix of real-time AI/ML steering during build and AI/ML steering of neutron experiments after the build
- Reuses AI/ML codes from 4D-STEM Experiments





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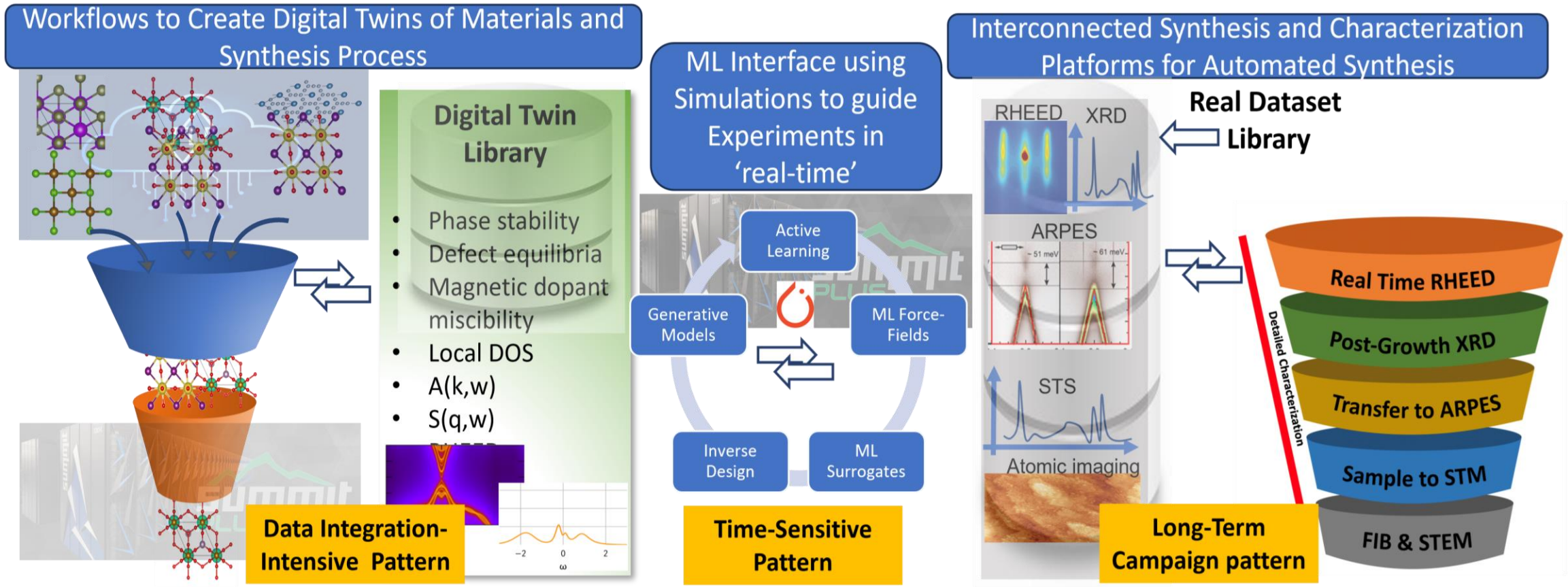
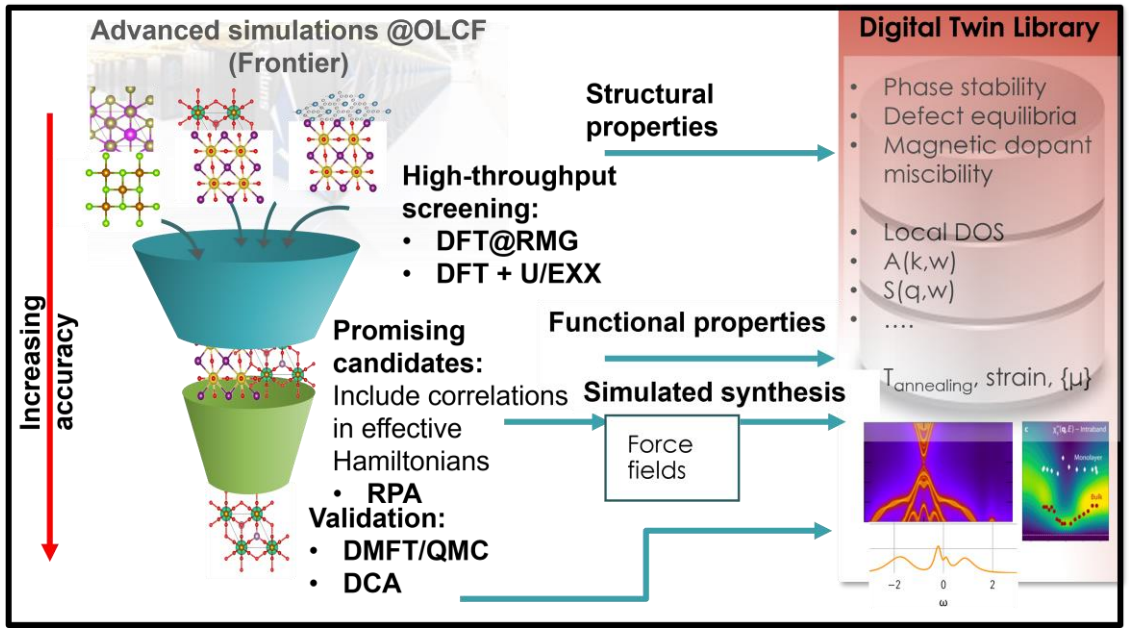
INTERSECT
INTERCONNECTED SCIENCE ECOSYSTEM

Autonomous Quantum Materials Theory + Synthesis + Characterization

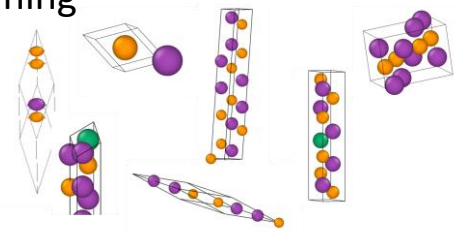
Quantum Correlated Materials Accelerated Discovery Platform (QCAD)



Hierarchical Computational Framework



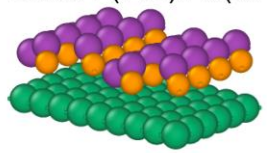
Heterostructure screening with incorporated heterogeneities



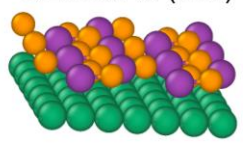
1. Deformation
2. Composition
3. Vacancies
4. Antisite
5. Interstitials
6. Substitution
7. Stacking faults

. . .

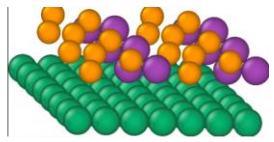
Bi3Se4 (101)/Nb(001)



Bi2Se3/Nb (101)



BiSe8/Nb (001)

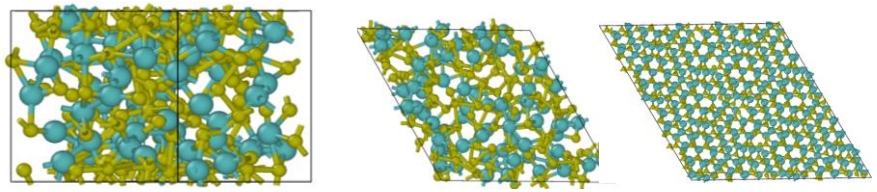


At various
- *Surface symmetries*
- *Substrates*
- *Heterogeneities*

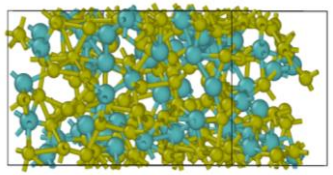
Generation of Digital Twin Synthesis and Property Library

At various
- *Temperature*
- *Strain*
- *Composition*
- *Quench-rate*
- *…*

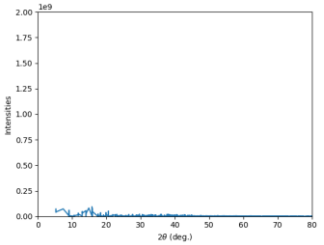
Final phases dependent on growth parameters



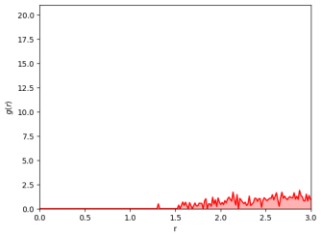
Structural transformation



Simulated XRD

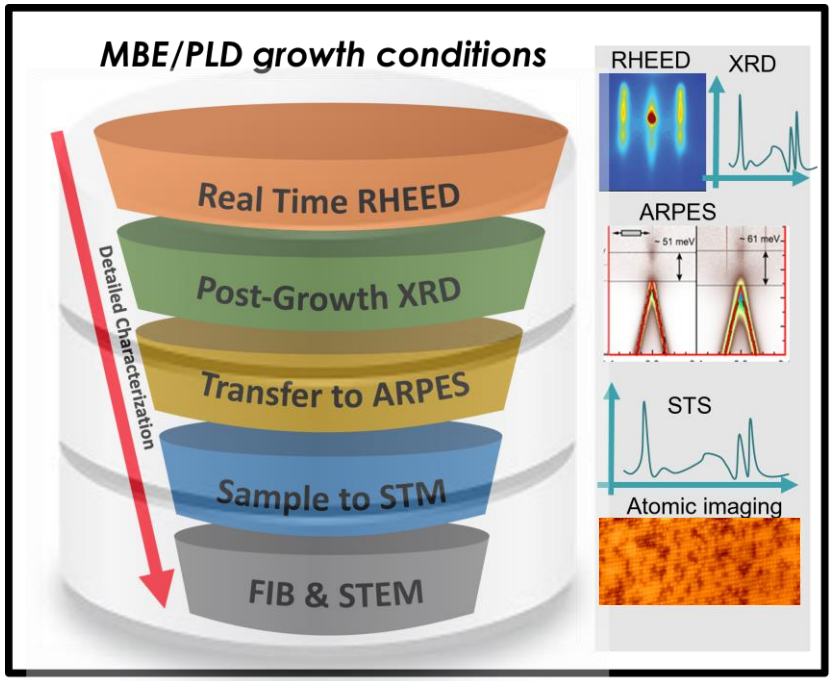


Pair Dist. Func.

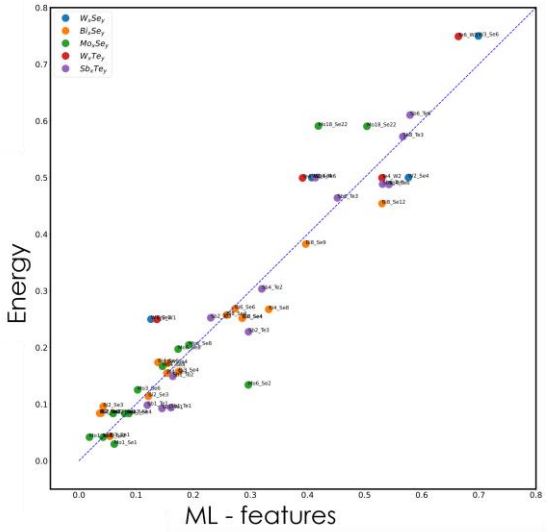


Maximizing computational efficiency for AI/ML workflows: Running ML and MD processes on GPUs and simultaneous post processing (XRD/RHEED/STEM/ARPES) on CPUs for every single compute node.

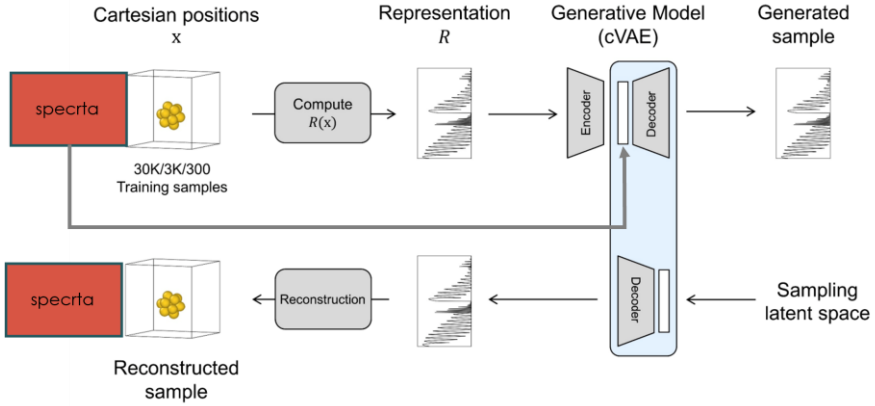
Theory-Experiment Co-Optimization



Energy correlation in feature-space

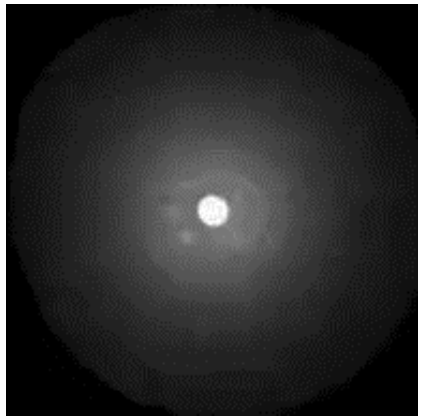


Experiment conditioned generative model

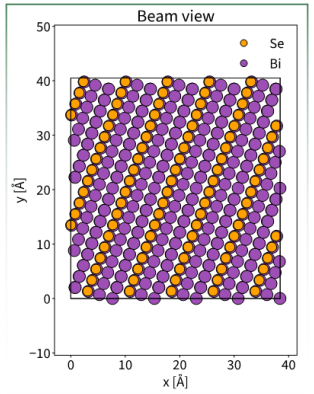


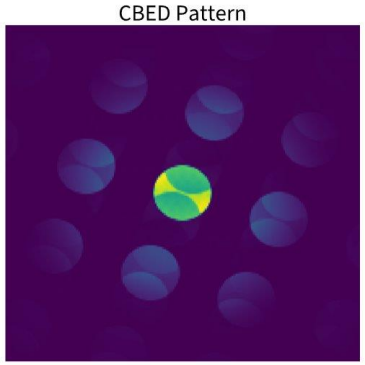
- Testing workflow on crystallization of topological and Transition Metal Dichalcogenide (TMDC) materials using the electron beam in a Transmission Electron Microscopy (TEM)
- Co-Optimization of theoretical and experimental Convergent Beam Electron Diffraction (CBED)

Experimental CBED pattern



Simulated CBED pattern from MD structures





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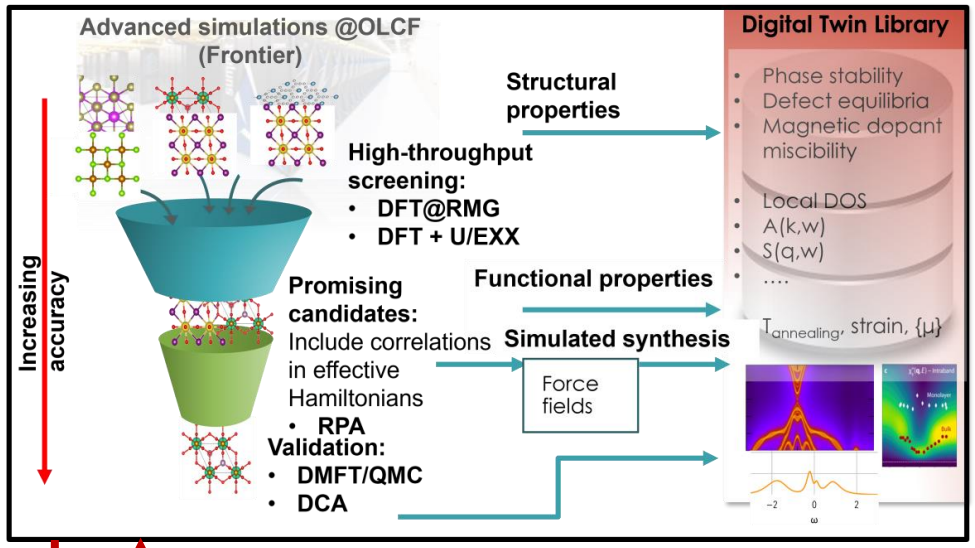
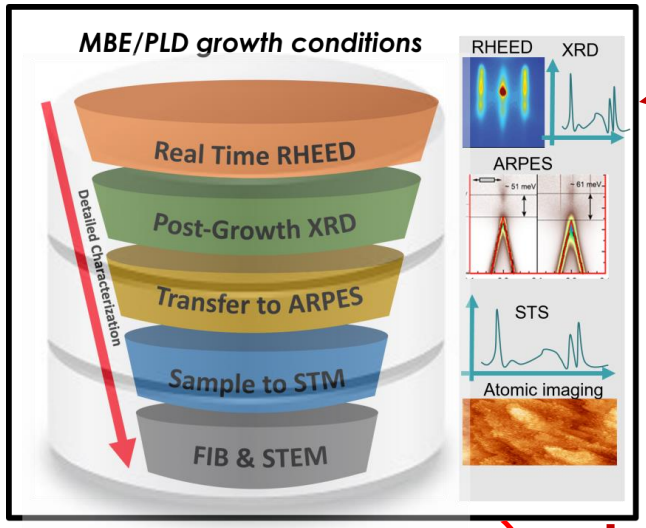
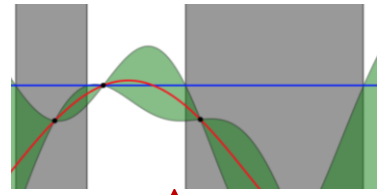
Physics-Driven ML Framework for Mulit-Modal Theory-Experiment Co-Optimization

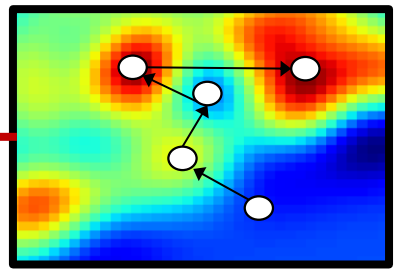




Automated modification of growth parameters to achieve desired properties



Bayesian Optimization

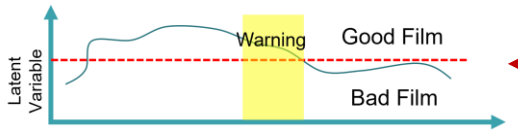


Generate new structures to screen for desired spectra

spec2struct

struct2spec (theory + expt.)

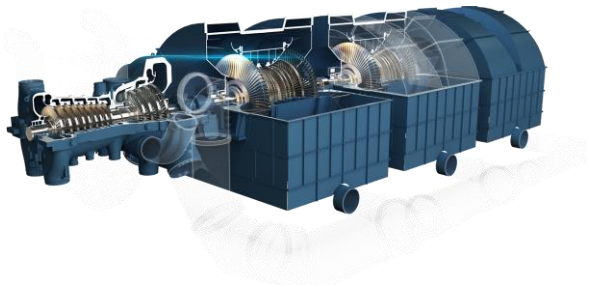
growth2spec

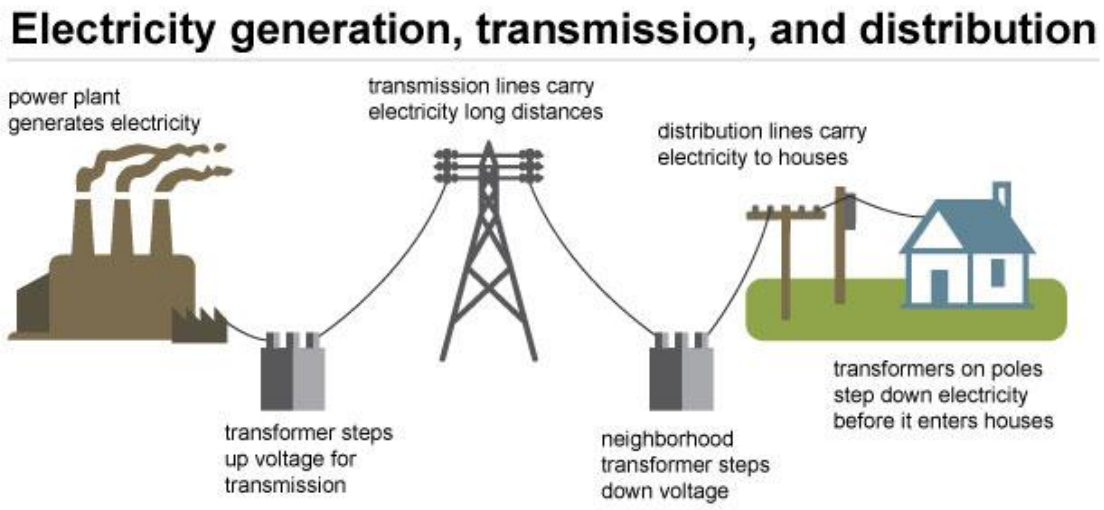


Real-time monitoring

Autonomous Electric Grid Optimization

The Electric Grid of Today





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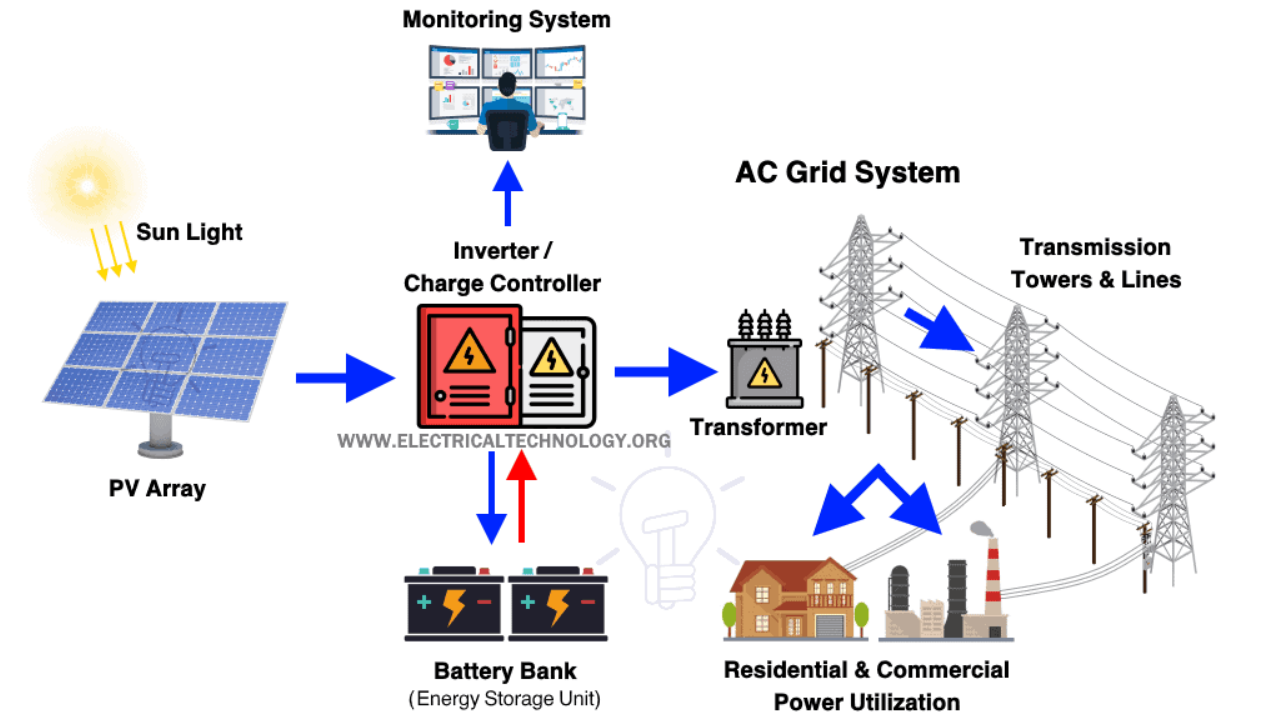
The Electric Grid of Tomorrow



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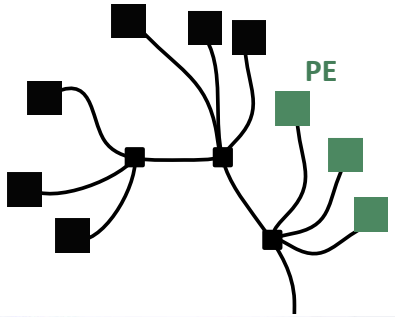
Electric Grid Modeling – The Old Way

Representative power grid with PEs

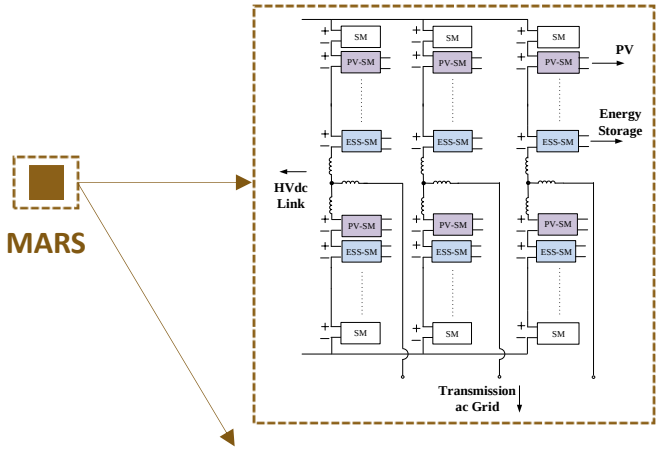


Step 1: Simulate power grid with PEs (without physical equipment or control node) in PSCAD based on data from MARS control nodes – DESIGN OF EXPERIMENT

Human-in-loop: Transfer data (non-real-time) to MARS control nodes from PSCAD simulations

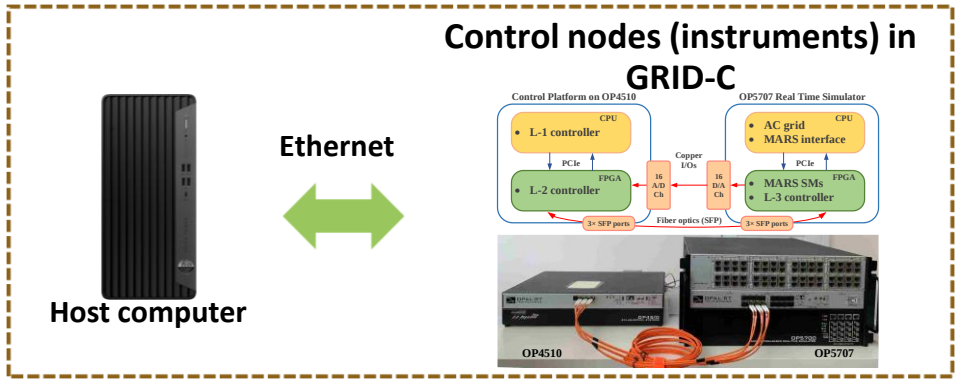
Human-in-loop: Transfer data (non-real-time) to PSCAD simulations from experimental runs

Multi-port Autonomous Reconfigurable Solar power plant



MARS, control nodes in GRID-C

Control nodes (instruments) in GRID-C



Step 2: Run MARS control nodes with the transferred data from PSCAD–EXPERIMENT

Iterative design of experiment and experimental runs needed for convergence in the above process to evaluate new real-world physical equipment – typical process time expected is of the ***order of several weeks for 0.25 second time steps***

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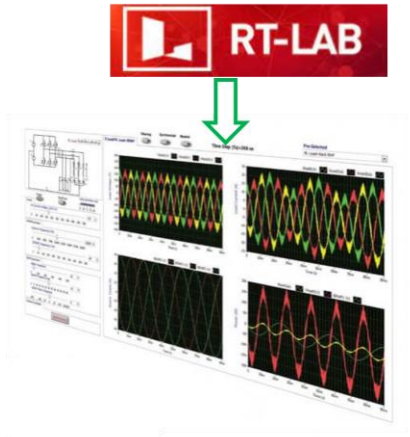
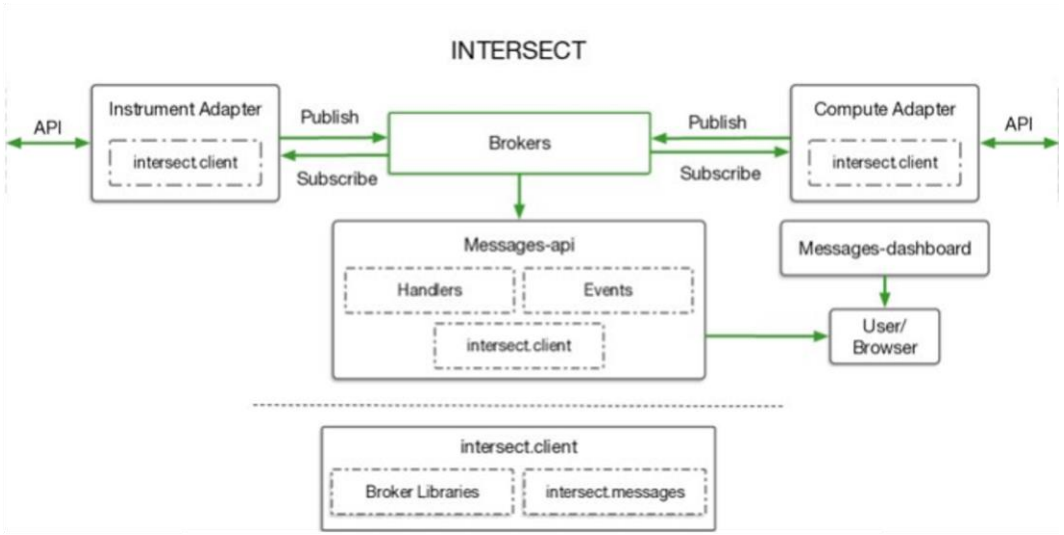
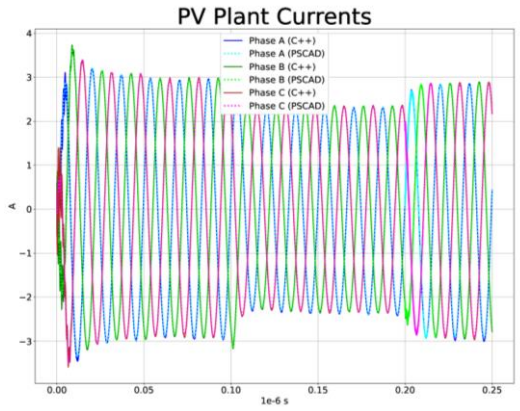
Electric Grid Modeling – The INTERSECT Way



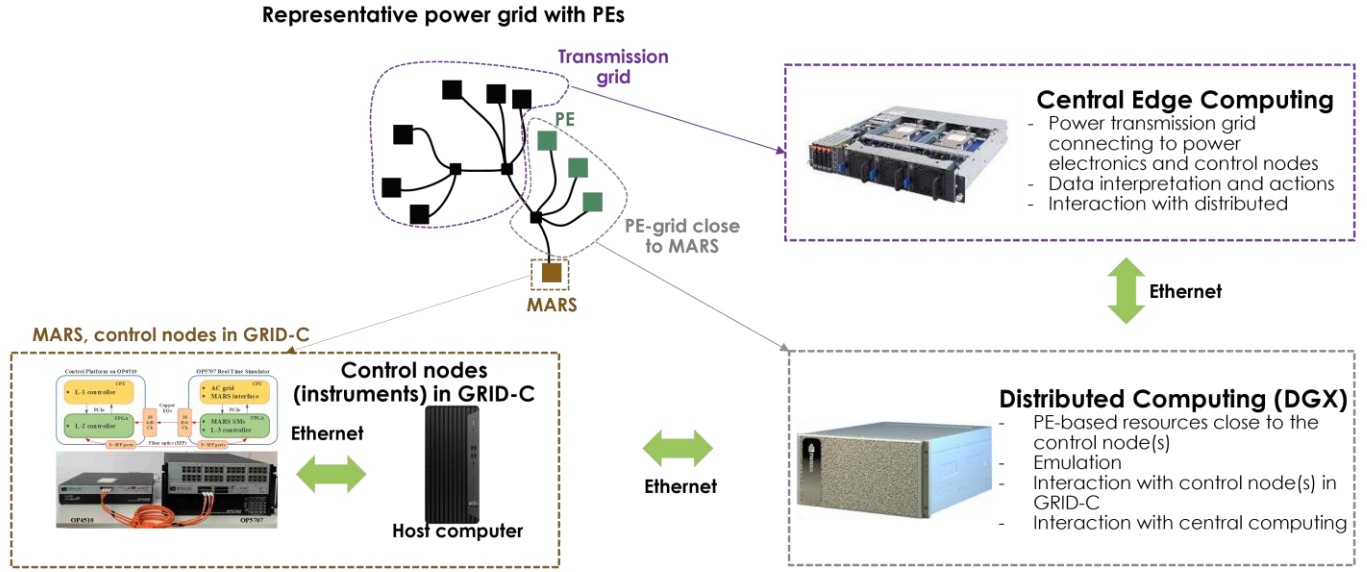




EMT simulation software (6221 nodes) running at 25 µs

- Different parts of the grid emulated on different computational resources based on proximity to the MARS
- Observe response of MARS power electronics as changes/disturbances are injected into the grid
- Latency is crucial for real-time emulation
- AI/ML optimizes power electronics parameters to increase grid reliability

Real-time optimization possible at 25 µs timesteps



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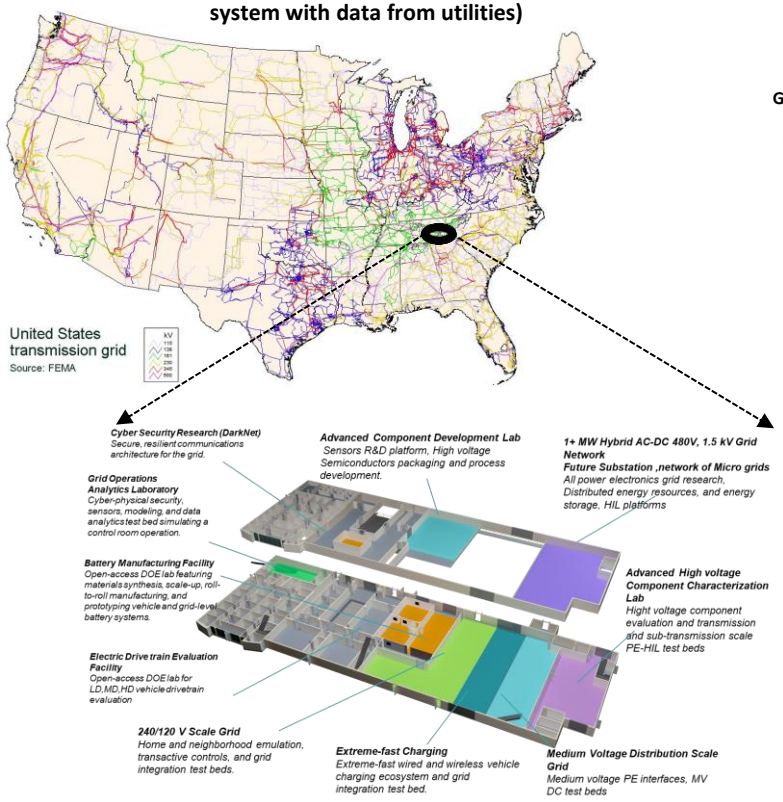
INTERSECT INTERCONNECTED SCIENCE ECOSYSTEM

Automation for Grid Interconnected-Laboratory Emulation (AGILE)

External Laboratory Connectivity
- Interconnected national laboratories
- Potential international connection

Ethernet (ESnet)

US energy system and power grid (real-world system with data from utilities)

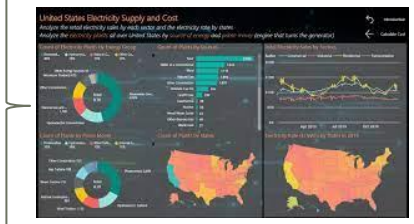


GRID-C laboratory at ORNL
- Physical equipment/control nodes

Grid data from real-world systems (eg, utilities)

Central edge computing
- Physics-based models (larger power grid)
- AI-based models
- Interface with laboratory computing resources
- Data interpretation and scientific observation (actions)
- Interaction with distributed computing

Data exchange with digital twinning of labs



Visualization dashboard

Data exchange with labs

Distributed computing
- Interface with real-time and central edge computing resources
- Interconnected laboratories
- Twin laboratory equipment with power electronics

Scalable Interconnected Laboratories for Large-Scale Connectivity and Real-World Energy Systems and Power Grid Emulation

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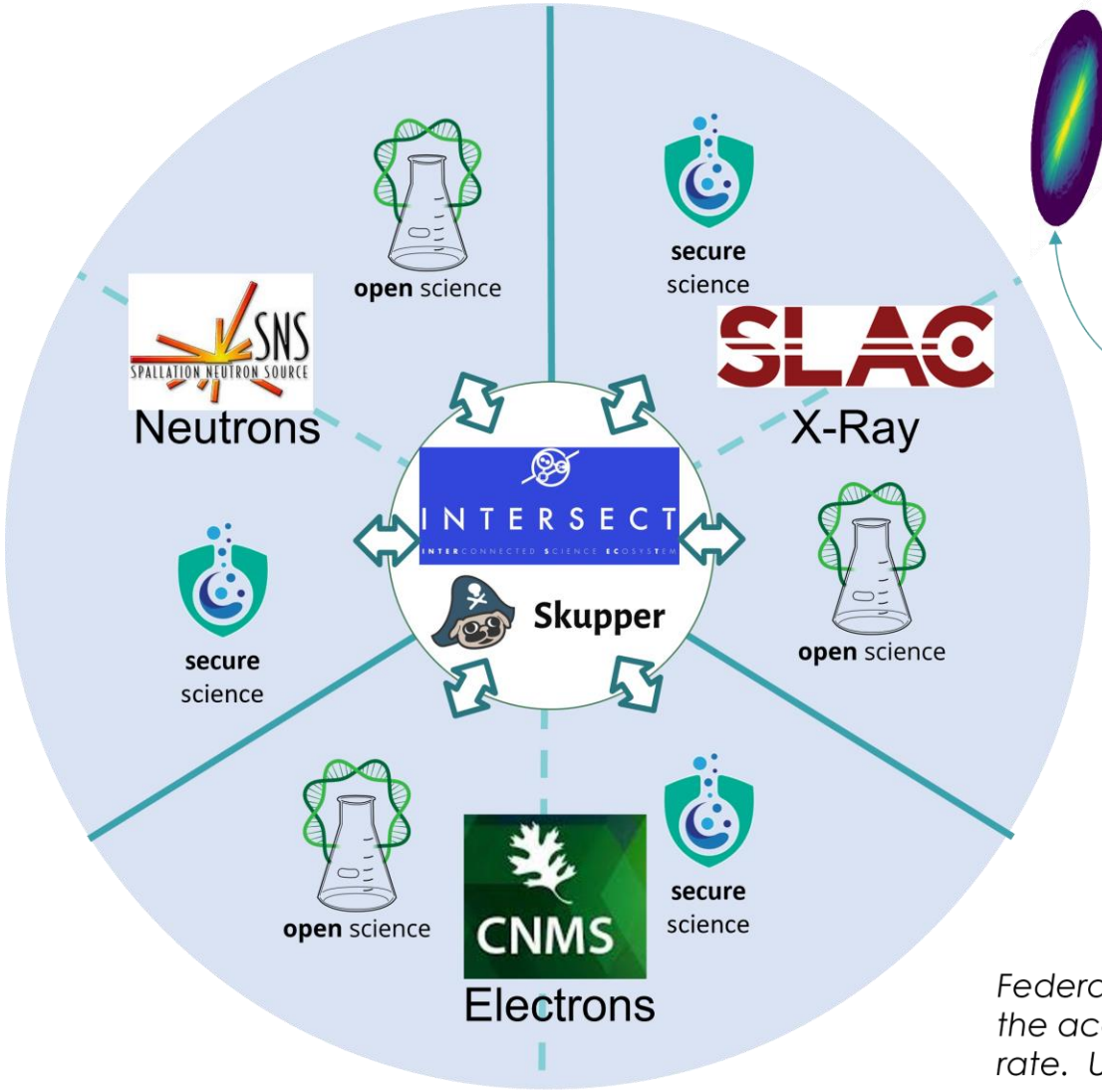
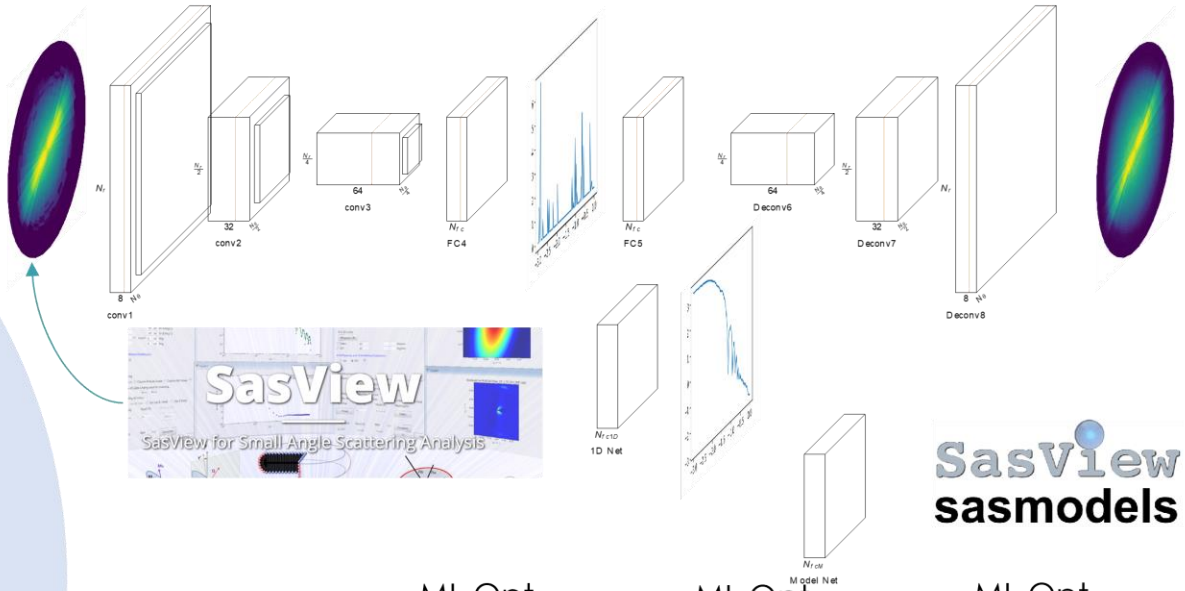
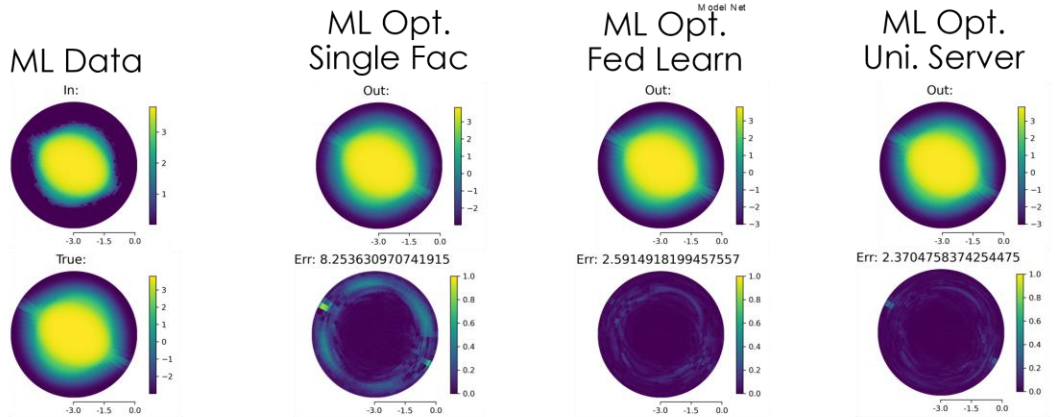
INTERSECT INTERCONNECTED SCIENCE ECOSYSTEM

INTERSECT – Beyond ORNL Borders

Federated Learning for Experimental Facilities (IBM/ORNL/RedHat/SLAC)



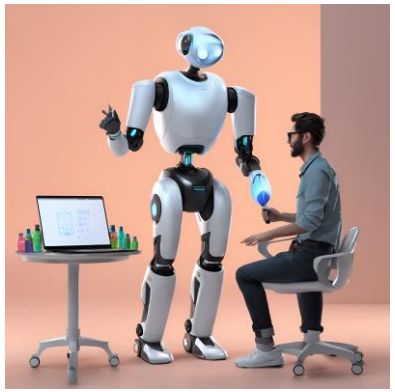
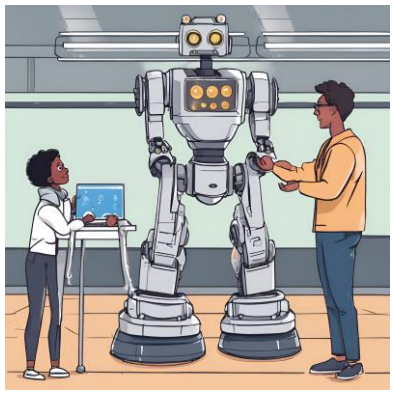




Federated Learning across different facilities and security domains increase the accuracy in reconstruction, model classification, and decompression rate. Using **SasView** *we build-in community based physical knowledge.*

Interconnected Science Ecosystem



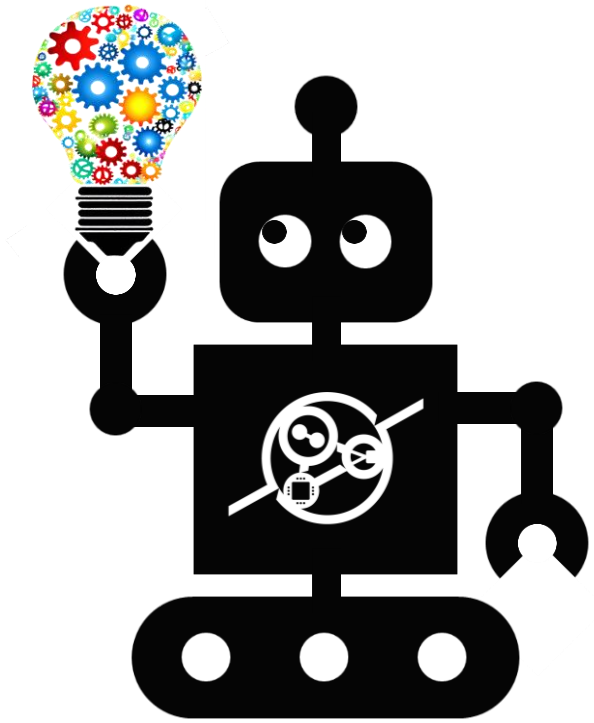



Community Engagement and Workforce Development are critical for Sustainability

- Open-architecture, open-source community-based development
- Mature microservices with standardized interfaces for interoperability
- Searchable code and data repositories
- Documented use cases and tutorials for quick deployment
- User friendly software development kits for quick adapter development
- Intuitive web portal for uploading and downloading resources

Lots of progress, but a long way to go!!

Questions?



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