FY23 LDRD

- Website: https://ldrd.lbl.gov/
- Timeline to remember:

FEB 11	A short presentation** to get initial feedback from the Division [≦ 5 slides with *preliminary* cost and staffing estimates && ≦ 10 minutes]
MAR 11	Final presentation** on the proposal to the Division [≦ 5 slides with *final/near-final* cost and staffing estimates && ≦ 10 minutes]
MAR 23	Proposal submitted to online LDRD system via the URL above
MAR 25	The Lab locks the submission website

****Zoom: https://lbnl.zoom.us/j/5104952467?pwd=Rno4VzJHTjlvTElrM3ZCZFR5bnlCZz09. Passcode: h9q62L8Y6f**

LDRD FY23

- Four tracks:
  1. **Lab-wide Initiative**:
     - Carbon Negative Initiative (CNI)
  2. **Early Career Development**
     - PhD no earlier than January 1, 2014
     - Applicant must have (or on track to) a scientific job title (career or career track, research scientist or staff scientist) before the project starts (October 1, 2022).
     - No more than 50% of the PI's overall time
     - $450,000 max (can be spread over 3 years)
  3. **Area-Priority** (next slides)
  4. **Multi-Area Topics** (next slides)

LDRD FY23 - PSA Area-Priorities

- High-risk projects with potential for significant impact are strongly encouraged :

  1. new scientific opportunities in particle physics and cosmology
  2. new opportunities in nuclear science ("*EIC and its detectors*" is explicitly mentioned)
  3. advanced accelerator systems for colliders and other applications including high power lasers
  4. novel technical concepts and capabilities: especially microelectronics, semiconductor detectors, quantum enabled technology, superconducting magnets
  5. novel computing capabilities including AI/ML applied to particle physics, cosmology, nuclear science and accelerators
  6. new opportunities in fusion energy sciences;
  7. leveraging LBNL capabilities to address national & homeland security mission needs, including monoenergetic photon sources, advanced neutron-based active interrogation concepts, and advanced radiation detection and imaging algorithms.

- Important Area priority:

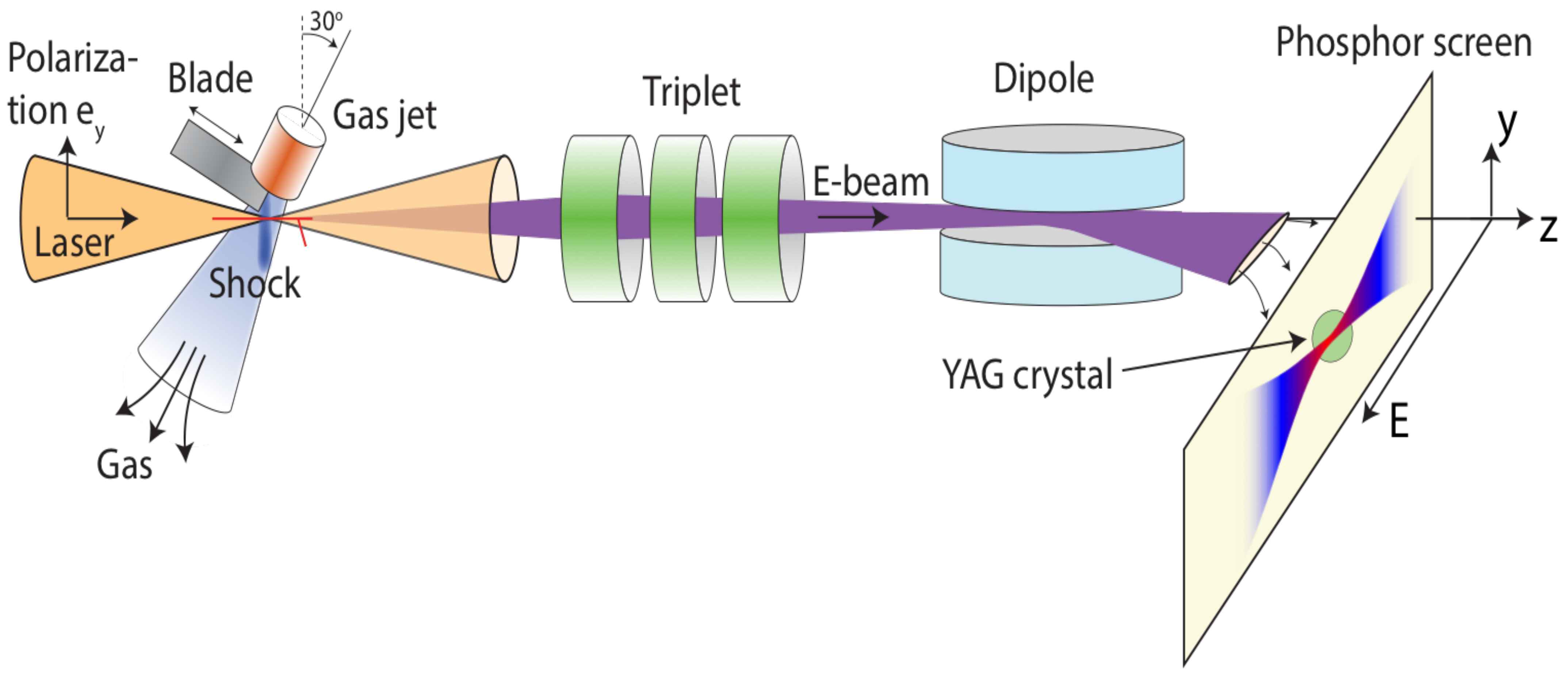
  FY23 is to support innovative ideas in instrumentation, with an emphasis on detector and readout R&D that could **enable scientific opportunities in more than one discipline**, with participation of multiple Divisions to create synergies across and outside the Area. Proposals may also include needed investments in technical infrastructure in support of instrumentation R&D.

LDRD FY23 - Multi-Area Topics

- Lead and co-PIs are responsible for co-planning work and budgets for each partner Area
- Funding will come from each of the researchers' home Area allocations with additional funds contributed by the Directorate reserve to support such projects. Funding splits will be determined on a project-by-project basis, depending on the technical contributions from each Area.
- The Directorate contribution will generally be limited to a maximum of $100K, although higher levels of funding may be possible in exceptional circumstances. Buy-in, communication, participation, and financial support is required from **all** Areas involved in any one proposal for the proposal to receive the additional Directorate reserve funding.
- **Three topics:**
  - Automation in the Acquisition and Management of Experimental Data (*Lab Automation, aka Self-driving Lab*) [Examples attached to this talk]
  - Data Science/Machine Learning to Accelerate Science
  - Instrumentation to Advance Fundamental and Applied Science

Self-driving accelerator controls and optimization methods

- Cross-cutting self-driving accelerator controls and optimization methods based on AI have the potential to advance the performance of particle accelerators ranging from conventional machines to a new generation of plasma-based systems that can offer increased performance in smaller facilities.
  - Berkeley Accelerator Controls and Instrumentation has recently demonstrated the capability of ML based self-tuning methods to improve performance in laser coherent combination
  - R&D on coupling AI-ML based self driven tuning with non-perturbative diagnostics to active feedback for laser pointing stabilization and other parameters is being carried out in the BELLA Center
  - Self driving feedback techniques offer analysis of in-situ magnet systems to improve control and design in the US Magnet Development Program

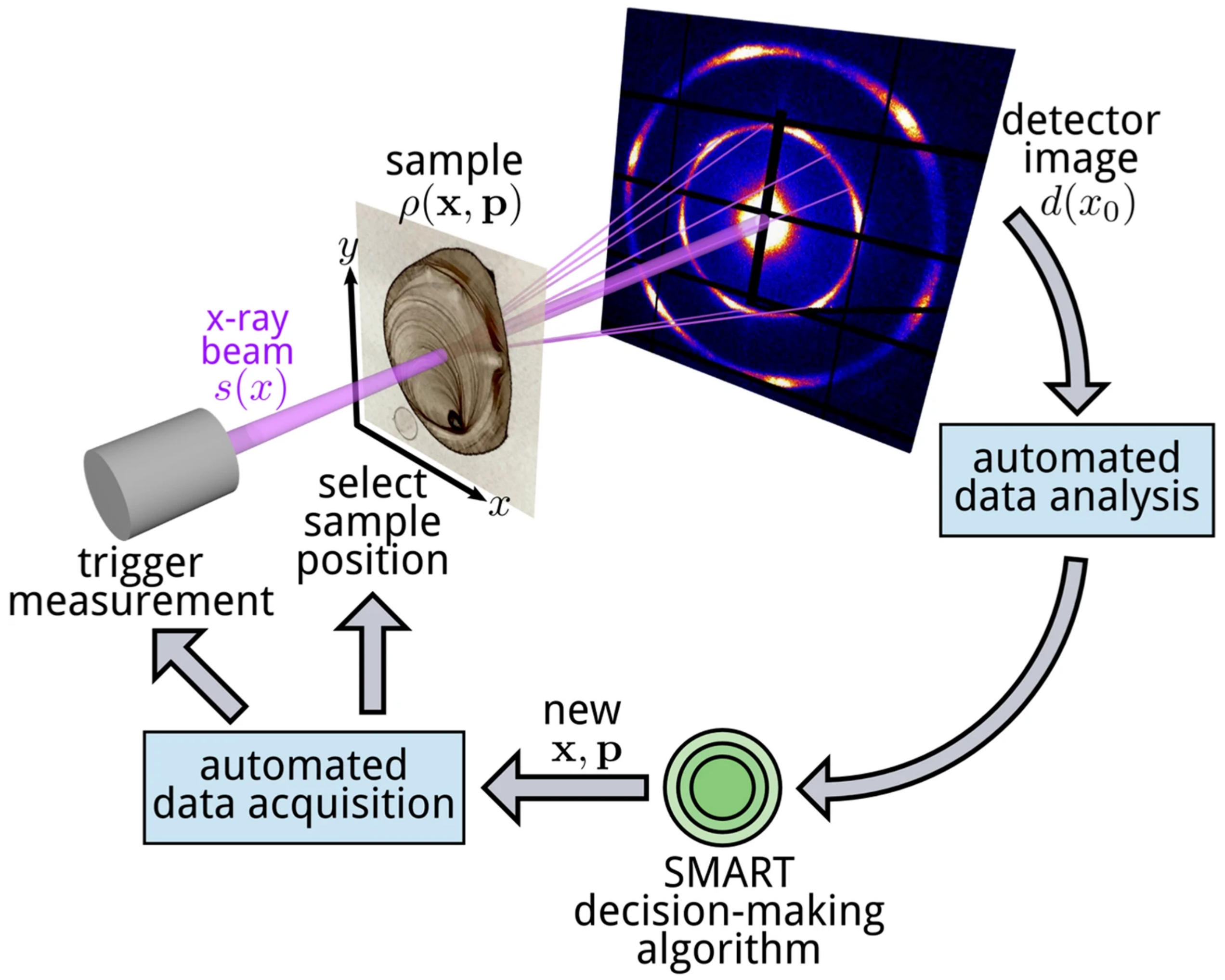


POC: Cameron Geddes (Accelerator Technologies and Applied Physics Division)

Other examples follow…

CAMERA and Autonomous Scientific Discovery

- Advanced Mathematics for Energy Research Applications (CAMERA) has developed and deployed AI-based autonomous discovery techniques across a broad scientific community.
- In April, a workshop on autonomous discovery in science and engineering sponsored by CAMERA attracted hundreds of scientists from around the world. https://autonomous-discovery.lbl.gov/
- Stochastic processes can be used to make decisions based on relatively small datasets, and they provide uncertainty estimates
- Application areas include: Autonomous driving of scanning probe instruments to map out and identify regions thin-film semiconducting systems; Investigating the thermal annealing history of DNA origami superlattices at the nanoscale; three-axis low-energy neutron scattering for the study of unconventional superconductors, low-dimensional and frustrated magnets and various quantum phenomena.



POC: James Sethian (Computational Research)

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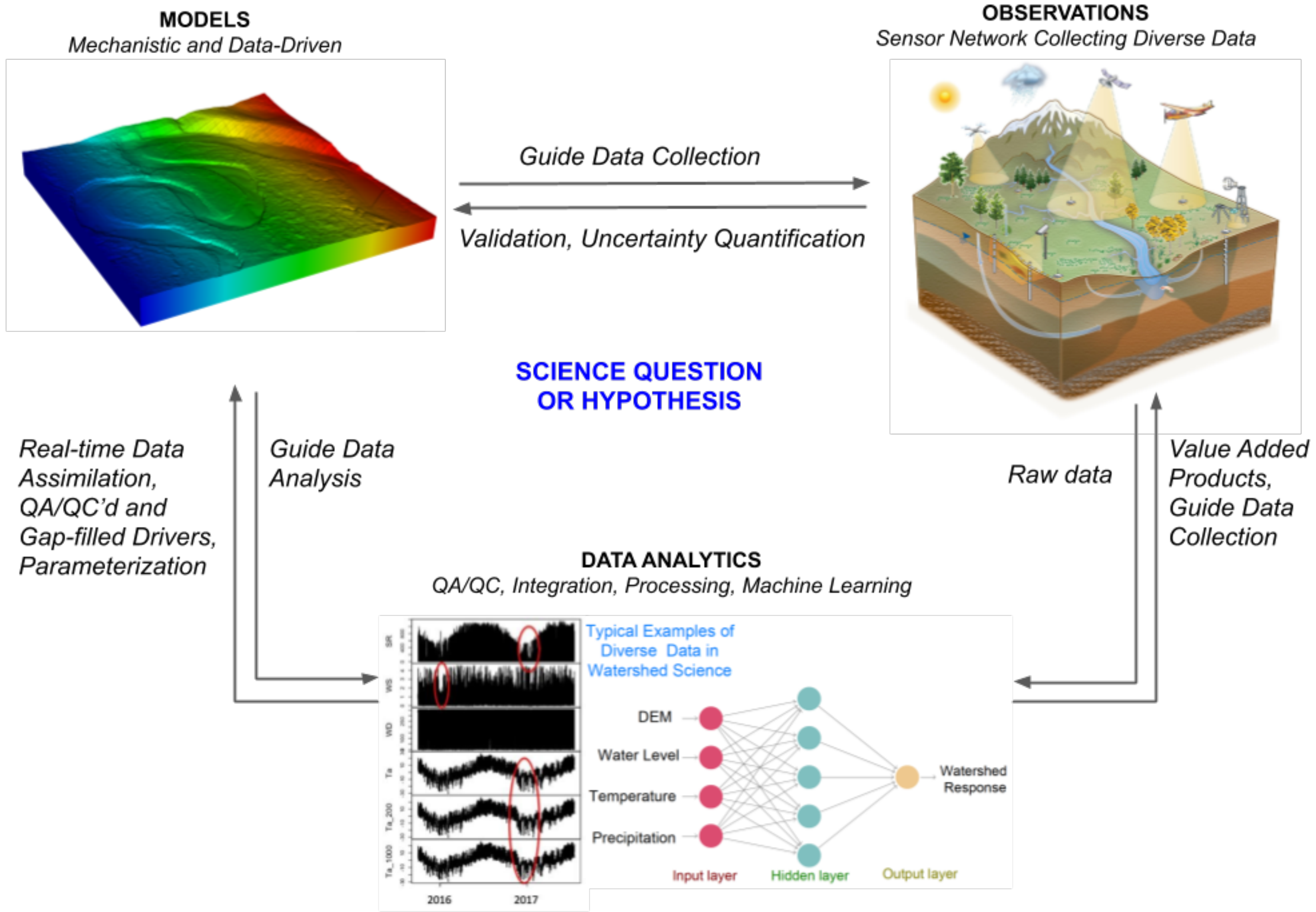
Self-Guiding Field Observatories of the Future

- Large amounts of diverse data are required to develop, parameterize, initialize, and validate regional to global land models
- Current data generated is still sparse and insufficient to capture the range, dimensions, and spatiotemporal heterogeneity of complex Earth system processes
- A Self-Guiding Field Observatory will include:
  - Models that drive automated data collection and experimentation
  - Adaptive, autonomous measurements in near real-time
  - Measurement technology innovations
  - Cyberinfrastructure to handle complex, dynamic data streams
  - Feedback of data into models and analytics



POC: Charuleka Varadharajan (Energy Geosciences)

EcoBOT: Automating Fabricated Ecosystems

- The EcoFAB project will create critical new insights into ecosystem processes through the creation of controlled model ecosystems in which microorganisms and host responses can be monitored in response to additional or changing variables.
- EcoBOT is an automated system under development to control growth conditions, refill and sample from EcoFAB media chambers, and image plants; providing liquid handling with a built-in custom growth chamber, imaging stations, and a robotic arm that integrates these components

POC: Trent Northen (Environmental Genomics & Systems Biology)

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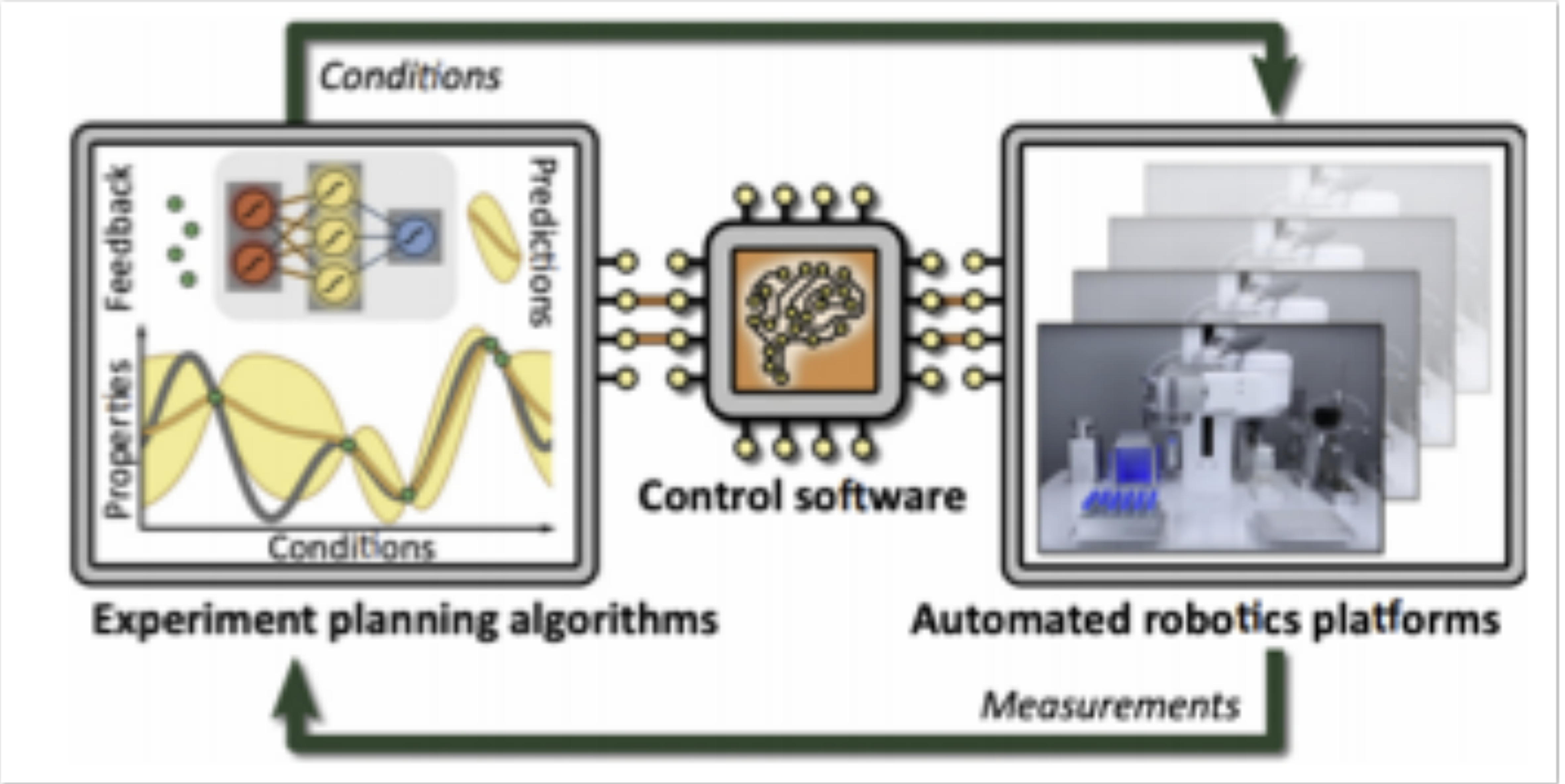
Self-Driving Labs for Predictive Synthetic Biology

- Recent advances in AI, synthetic biology and microfluidic platforms bring the potential for fully automated labs to produce the abundant high-quality data needed for predictive synthetic biology.
- AI can be used to automate the sequential design of experiments, including the discovery and refinement of hypotheses. Systems would collect information from the available scientific literature and combine it with the experimental results obtained from the self-driving labs.
- Leveraging novel reporting and summarizing capabilities in AI, self-driving labs will enable humans to develop hypotheses and interpret results, while facilitating experimentation that optimally explores all available pathways to achieve a desired target.



Self-driving laboratories couple automated robotics platforms for experimentation and data collection, with AI systems that choose not only the parameters for the next experiment but also the hypotheses to be tested

POC: Hector Garcia-Martin (Biological Systems & Engineering)

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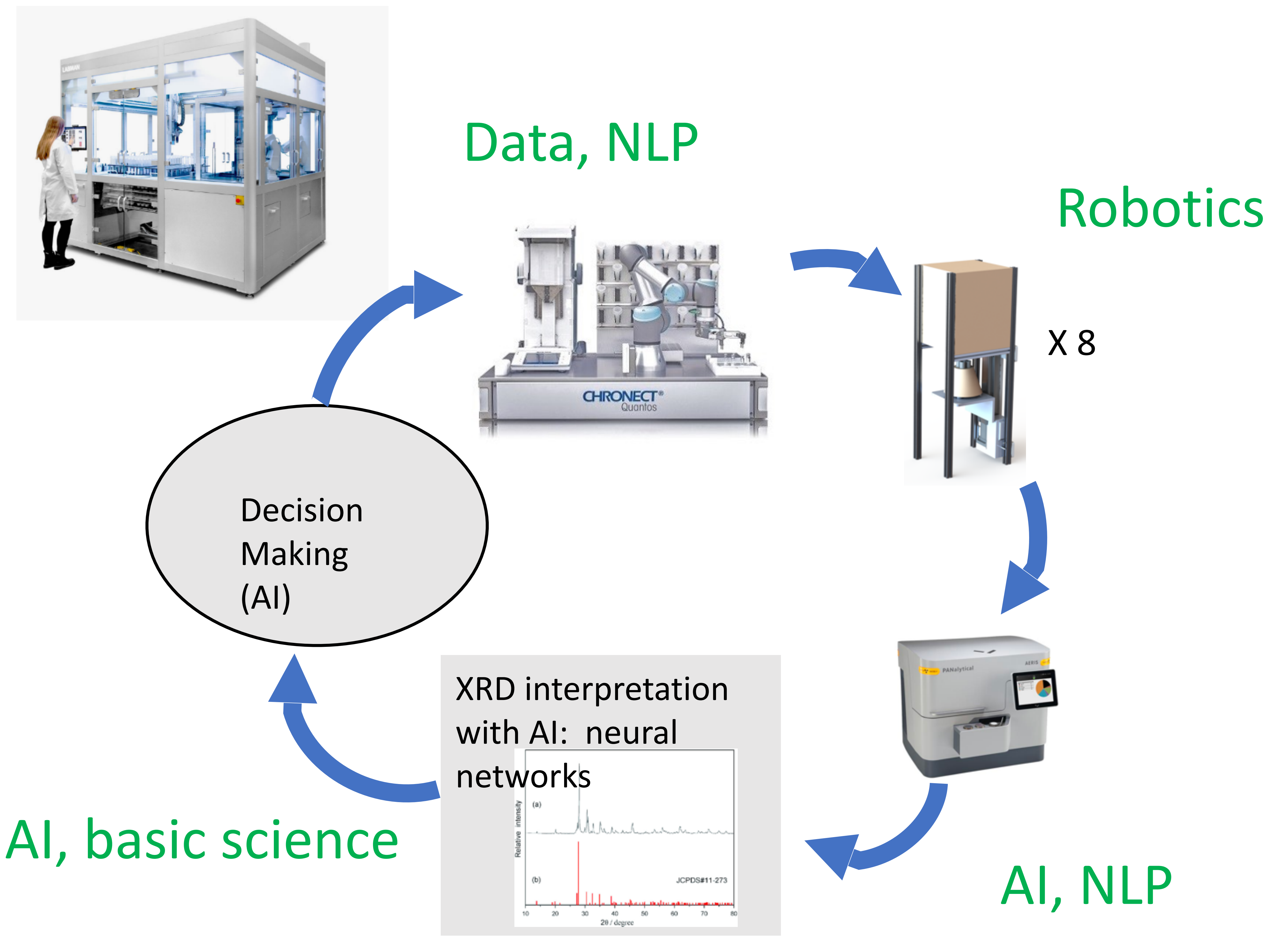
An AI-powered Autonomous Laboratory for Materials Synthesis

Motivation

- Computational design of novel energy storage materials has become very good, making the bottleneck the synthesis of novel compounds
- Synthesis and characterization of materials is slow and has not yet benefited from automation and AI

Objectives

- Create a fully autonomous lab for the synthesis of novel inorganic solids where ML is used for data interpretation and decision making (closing the loop)
- Integrate AI/ML with historical synthesis data, already extracted by the team from 5 Million research papers using Natural Language Processing (NLP)
- Perform materials synthesis at least 50x faster than in a traditional lab
- Demonstrate success on energy storage materials



Equipment choices tuned to achieve balanced throughput

Fully autonomous oxide synthesis facility

Target: 24 iterations per 24hr

POC: Gerd Ceder (UC Berkeley and Energy Technologies Area)