Brookhaven National Laboratory

U.S. DEPARTMENT OF ENERGY

Anomaly detection, predictive maintenance & facility optimization for Scientific Discovery by Human-AI-Facility Integration

Primary Investigator: *Vincent Garonne (NPP)*
Other Investigators: *Jerome Lauret (NPP), Qiulan Huang (NPP), Xin Dai (CSI), Ai Kagawa (CSI), Kevin Brown (CAD)*

6/1/2022

FY2023 NPP LDRD Type A Proposal

Proposal title: ***Anomaly detection, predictive maintenance and facility optimization for Scientific Discovery by Human-AI-Facility Integration***

Primary Investigator: ***Vincent Garonne (NPP/SDCC)***

Other Investigators: ***Jerome Lauret (NPP), Qiulan Huang (NPP), Xin Dai (CSI), Ai Kagawa (CSI), Kevin Brown (CAD)***

Ongoing discussion with NSLS

Indicate if this is a cross-directorate proposal: ***Yes (Submitted by NPP)***

If yes, identify other directorates/organizations: ***CSI, CAD***

Program: ***Multiprogram***

Proposal Term: ***3 years*** From: ***Oct, 2022*** To: ***Sept, 2025***

Total funding per year in FY23, FY24 and FY25: ***$400K/y***

Description of the LDRD Proposal

Project Description:

- The goal of the project is to ***build an intelligent system*** that provides ***anomaly detection, predictive maintenance and optimisation*** for ***large scientific instruments*** such as Accelerators (CAD/EIC, NSLS), computing centers (SDCC) or large arrays of sensors
- ***SDCC will host the computing architecture to perform the analysis of data, anomaly detection and intelligent autonomous control***

Main Goals:

- ***Detect anomalies and non-optimal setups***
- ***Predict imminent failures***
- ***Provide adaptive feedback and actions***

The priority research direction motivating this proposed work:

"Discovery Science Driven by Human-AI-Facility Integration"

Addressed research topics in this proposal:

1) AI enhanced detectors, accelerators, and sensors
2) Optimal experimental design and steering
3) Migration to operation

Large Scientific facilities: An ever growing complexity

Large scientific facilities are ***difficult to operate and optimize*** as they have many complex and interdependent components

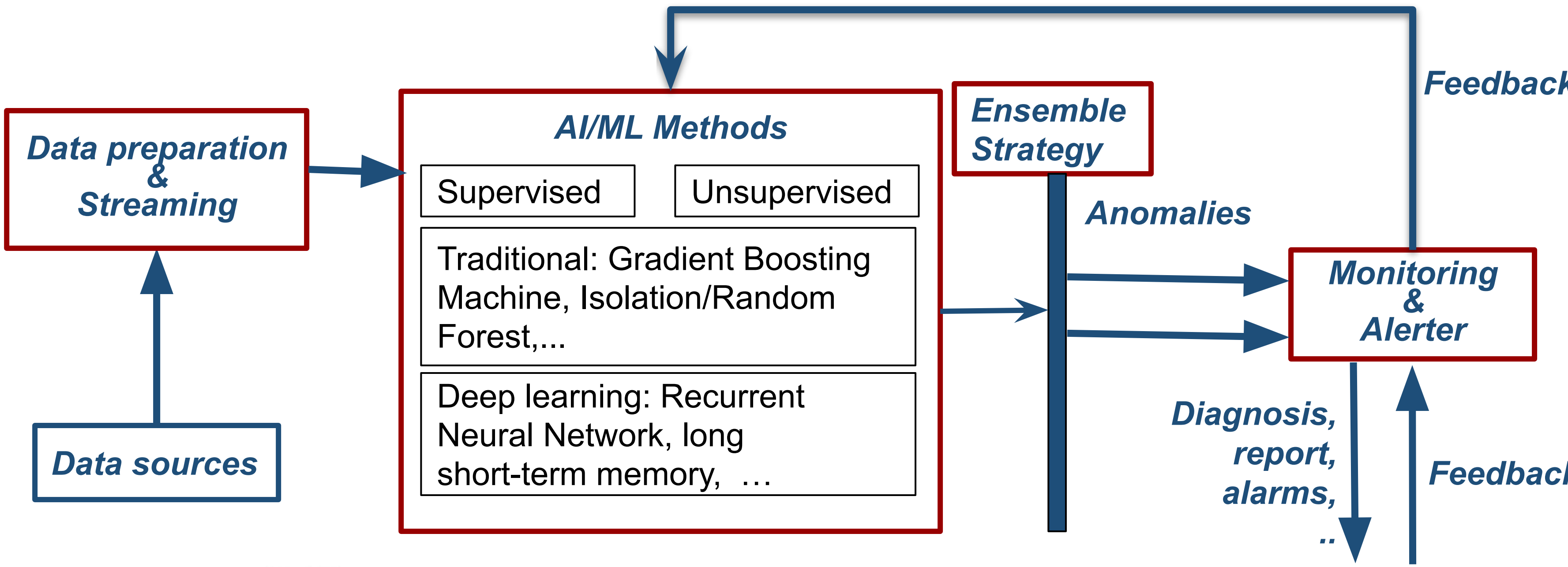
- ***Accelerator / Controls Systems***
  - Hundred of thousands of monitoring devices (sensors and control variables)
  - Monitoring a single sensor or control variable without classifying or correlating observed behavior with the behavior of other devices is insufficient to properly detect anomalies in complex systems
- ***SDCC — Similarities in the complexity compared to an accelerator***
  - Hundred of thousands of devices (20k spinning disks, 100k compute cores, ~500 GPU cards with Millions of jobs.day-1, several Millions of files created/ deleted/transferred.day-1, traffic at 100 GB/s)
  - Independent monitoring for each system is insufficient to properly detect anomalies — rely on staff awareness and root-cause investigations

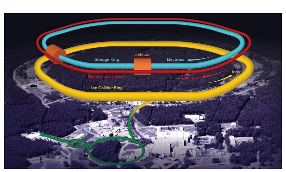
The evolution with the rapid adoption of new bleeding-edge technologies keeps increasing instrumental complexity and operational cost

- ***SDCC:*** Over the next five years (before HL-LHC anticipated for 2030) the size of SDCC will increase by an order of magnitude, adding to an already growing resource demands from NP programs under constrained size of effort
- ***Accelerator / Controls Systems:*** Significant effort is spent on tuning and optimizing the control variables of accelerators to minimize beam losses while maximizing beam quality for the experiments. Such systems do not scale easily to large numbers of variables

⇒ Scaling issues soliciting the use of AI/ML methods

Anomaly Detection - Architecture





Accelerator(s) *SDCC*

Domain experts

Data analytics pipeline:

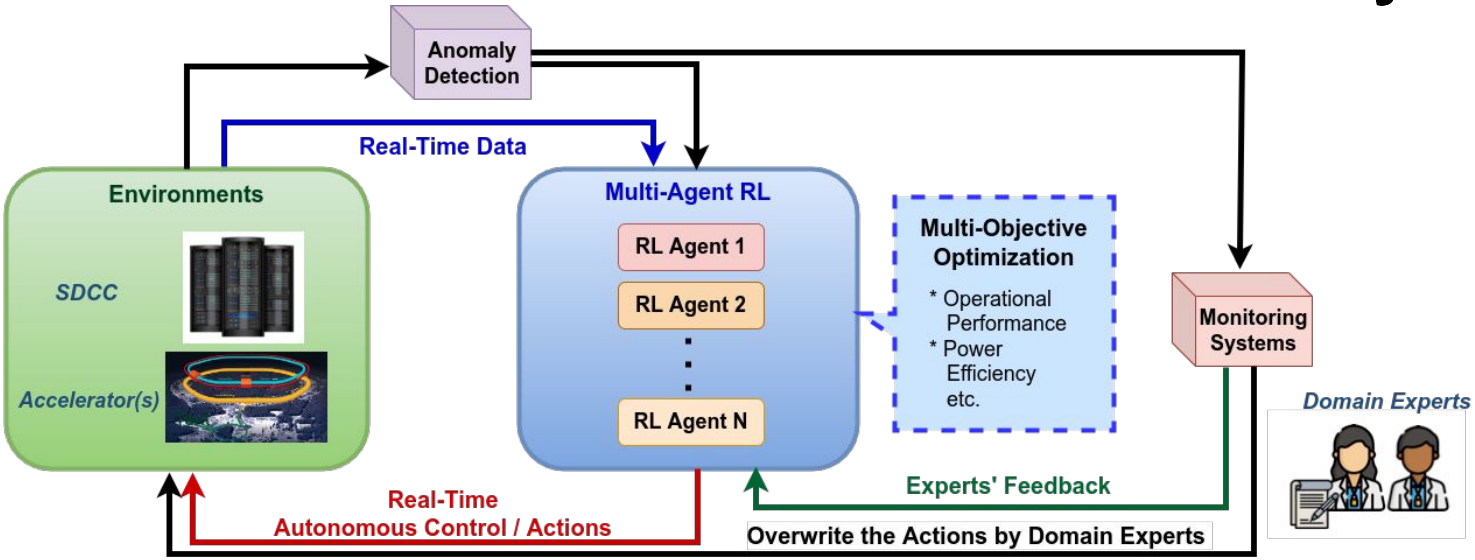
- Extract Transform Load, streaming, ..

Annotation pipeline:

- Label data, log clustering, create benchmark dataset, ..

— Proposal contributions

Intelligent Autonomous Control with Human-AI-Facility Integration



Goal: Develop **a novel multi-agent and multi-objective Reinforcement Learning (RL) algorithm** to improve intelligent and autonomous control along with anomaly detection and monitoring systems for **Human-AI-Facility integration**.

Limitation 1: Limitation to carry out autonomous control for realistic large-scale facility resources using real-time big data

Solution: Develop a novel **multi-agent RL algorithm** to effectively coordinate scientific resources and improve the scalability of our RL algorithm.

Limitation 2: Lack of ability to jointly optimize multi-objectives (various evaluation metrics) to improve the performance of a large scientific facilities

Solution: Design a novel **multi-objective RL algorithm** to **jointly optimize multi-criteria** (i.e. operational performance and power-efficiency) for scientific facilities.

Limitation 3: Inability to efficiently execute real-time implementation of ML training and ML-enhanced autonomous controls for large scale scientific facilities with human-in-the-loop AI approach

Solution: Experts from SDCC, MLG, and CAD will collaboratively conduct experiments to investigate the **optimal real-time execution of the human-in-the-loop-AI-integrated system** for **scientific facilities.**

Methods & Technologies

We will take an iterative, agile and co-design delivery strategy:

Activity 1. Data analytics pipeline (M18*)

SDCC: Qiulan Huang, Vincent Garonne, Jerome Lauret, ***CAD:*** Kevin Brown

Activity 2. AI/ML models, algorithms & implementation (M24*)

CSI: Xin Dai, Ai Kagawa

Activity 3. Visualization & Alerter (M36*)

SDCC: Qiulan Huang, Vincent Garonne

Activity 4. Scientific Use cases (SDCC, EIC, NSLS, ..) gathering and demonstration of the system's capabilities (M36*)

SDCC: Jerome Lauret, ***CAD:*** Kevin Brown

* Cf. Gantt Chart on slide 11

We will exploit the rich set of tools of the SDCC monitoring, data analytics infrastructure and leverage the SDCC expertise

Funding Requirements

Total funding per year in FY23, FY24 and FY25: $400K/y

Total FTEs: Between 1.5 and 2

Team & Roles

SDCC: High level Scientific and Information technology experts

- Vincent Garonne (PI, SDCC)
- Jerome Lauret (Science use cases / Advisor, SDCC)
- Qiulan Huang* (Data collection infra./analytics, SDCC)

CSI: Artificial Intelligence and Machine Learning experts

- Xin Dai* (Large-scale data analysis, online anomaly detection, CSI)
- Ai Kagawa* (AI/ML using HPC, reinforcement learning, CSI)

CAD: Accelerator & Controls Systems experts

- Kevin Brown (Science use cases / Advisor, CAD)

* Eligible for early career awards

Summary (1/2)

Our proposal is well responsive to the FY 2023 LDRD strategic plans: ***"Discovery Science Driven by Human-AI-Facility Integration" — Topics: 1, 2 & 3***

- Add value for various programs in NP & HEP, CSI, CAD/EIC, NSLS
- Collaboration & synergy between departments and teams

It offers a timely opportunity to bring large scientific facilities to the next level of intelligent and autonomous facilities

- ***Prognostics:*** Detecting anomalous behavior will improve our ability to prevent failures, increase availability and improved feedback loop
- ***Optimization:*** Tuning and optimizing their usage, e.g., control variables of accelerators tuning can minimize beam losses while maximizing beam quality for the experiments
- ***Modeling:*** The state-of-the-art AI/ML solution developed in the project can be applied to other facilities

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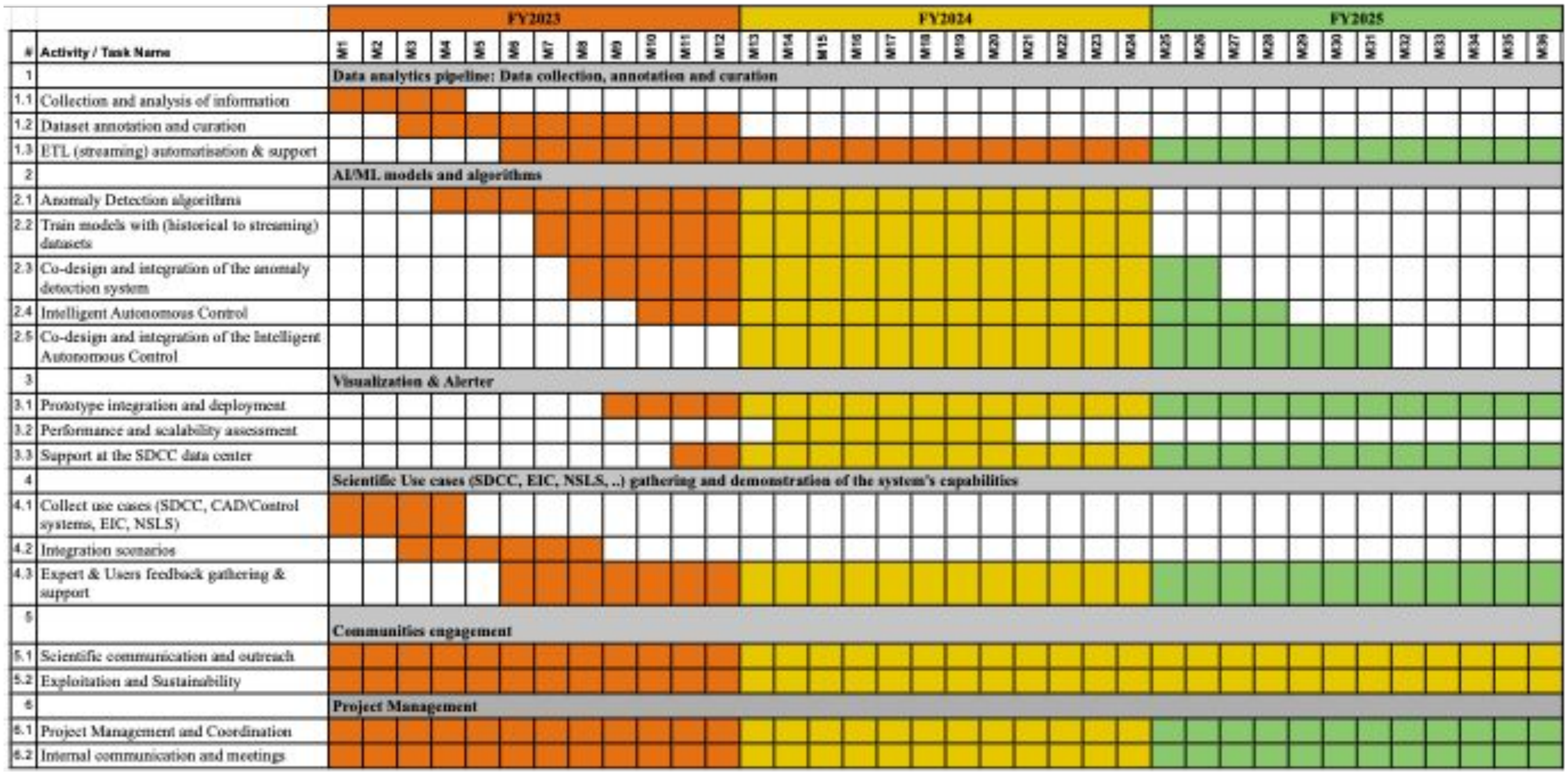
Summary (2/2)

Return on Investment

- ***SDCC:*** Expected enhanced stability and uptime will have a net beneficial impact to a large base of Scientists and Scientific programs — While growing by an order of magnitude on hardware with workforce discrepancy
- ***CSI:*** Topics for research in Artificial Intelligence and Machine Learning which will produce scientific e-science/AI publications in Peer-reviewed journals/IEEE conferences
- ***CAD:*** More intelligent methods will give us an edge in predicting faults by allowing us to act preemptively to minimize beam losses while maximizing beam quality and improve availability for the experiments

⇒ Increase up time by early detection of anomalies
Save $$ for the long term with common solutions

Gantt chart



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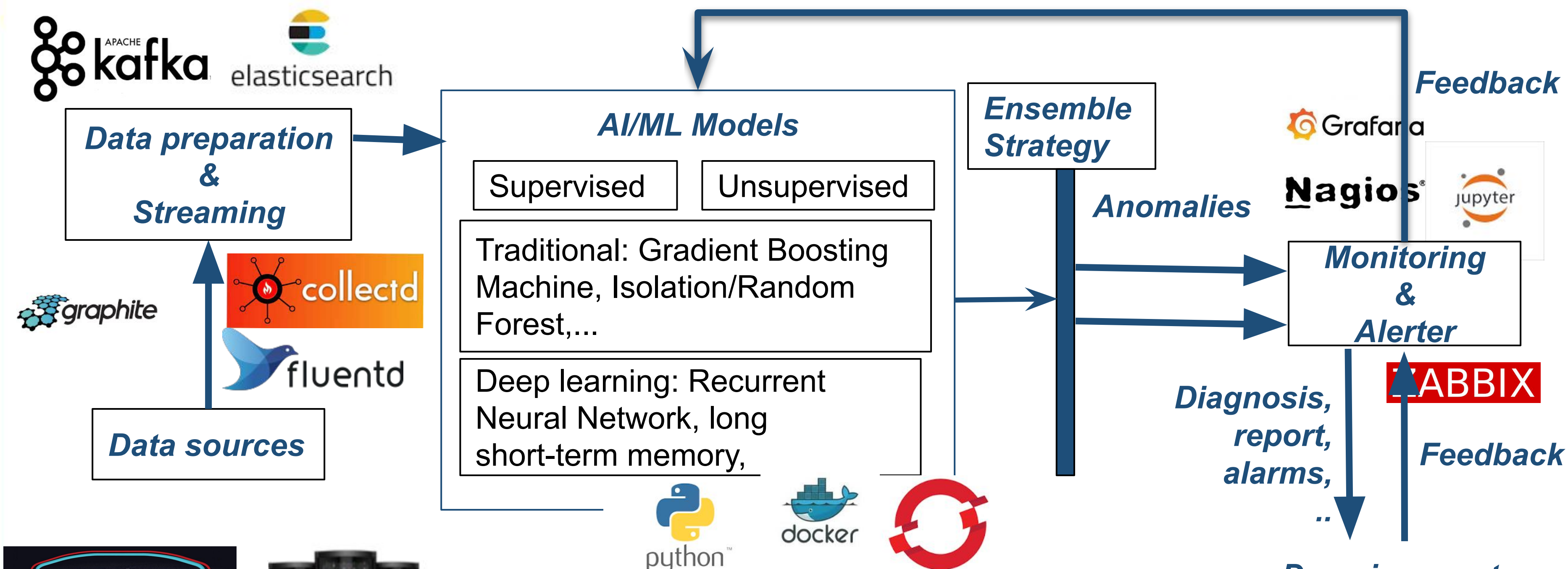
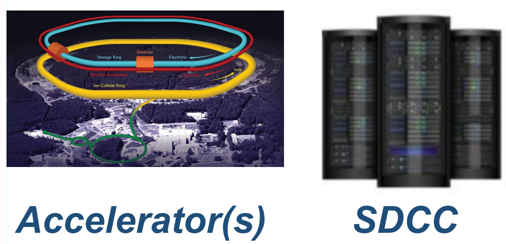
Anomaly Detection System - Architecture





***Prognostics*:** detecting anomalous behavior will improve our ability to prevent failures and increase availability
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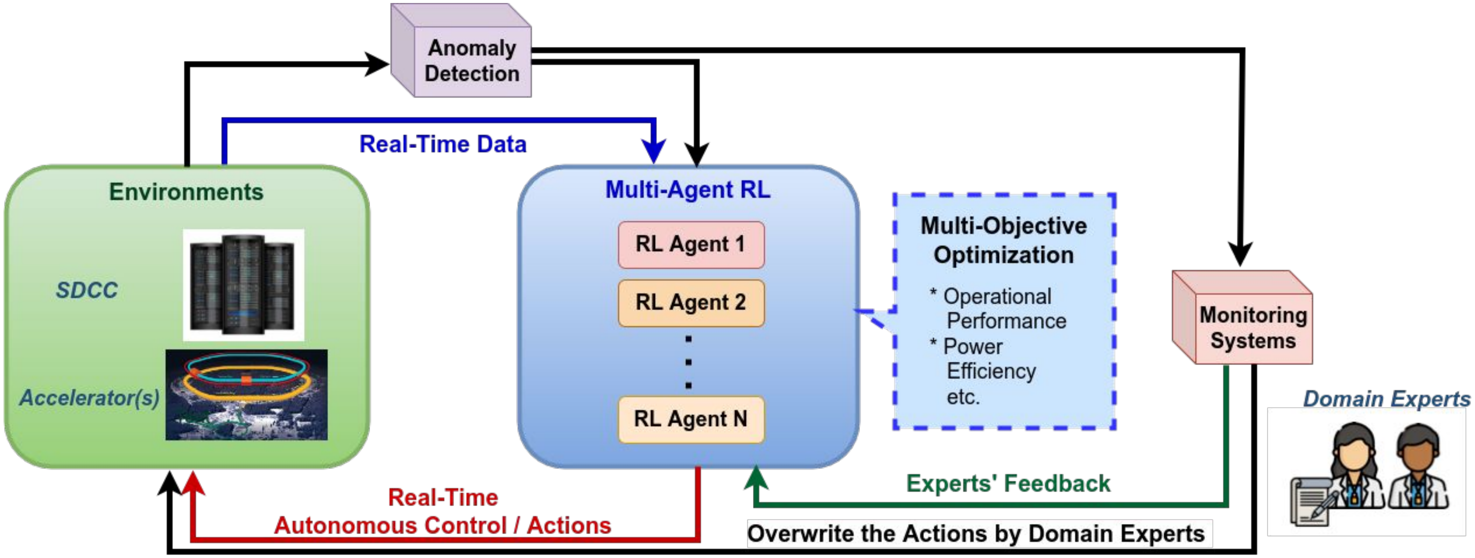
Backup Slide:
Intelligent Autonomous Control with Human-AI-Facility Integration



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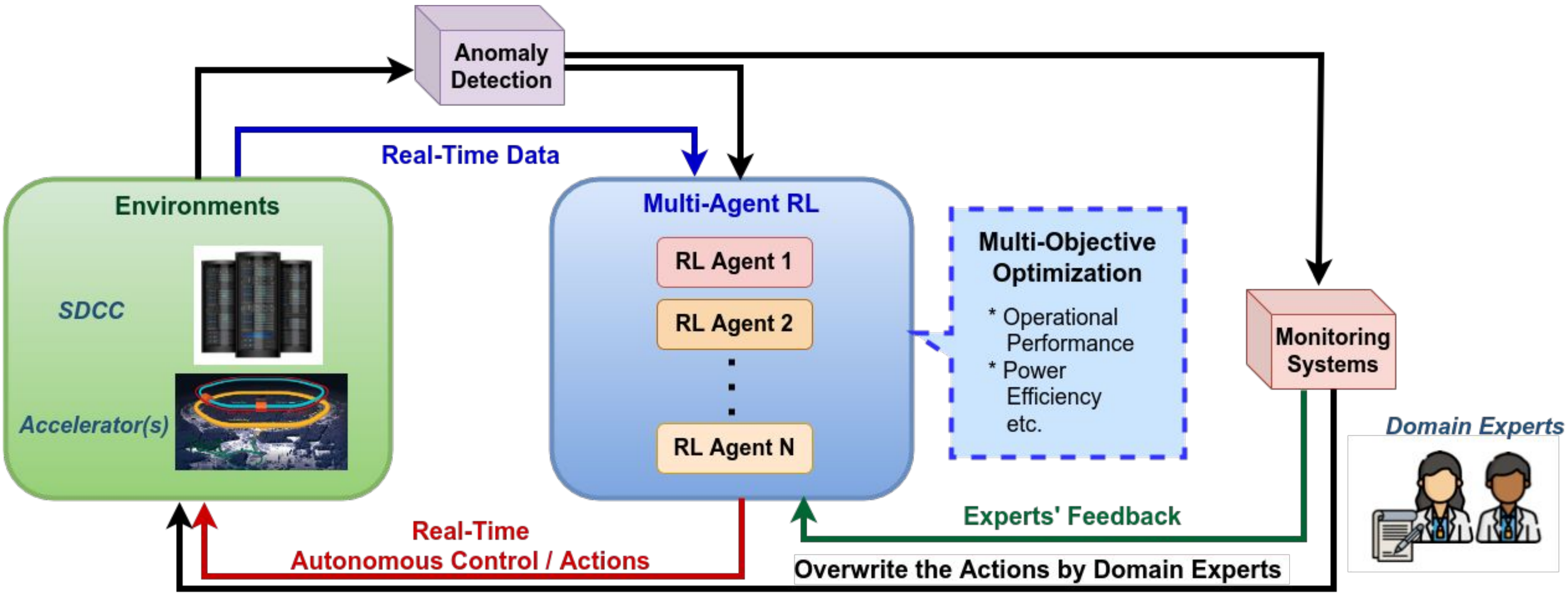
Intelligent Autonomous Control with Human-AI-Facility Integration



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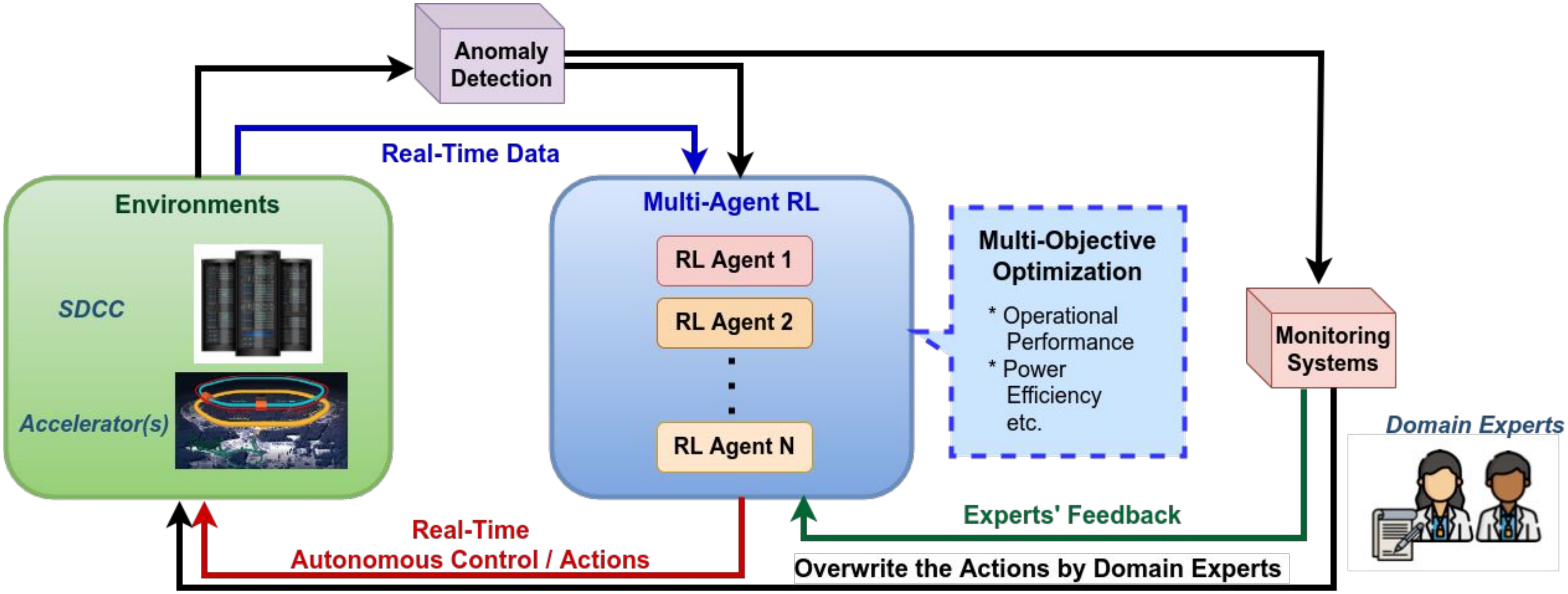

Limitation 1: Limitation to carry out autonomous control for realistic large-scale facility resources using real-time big data

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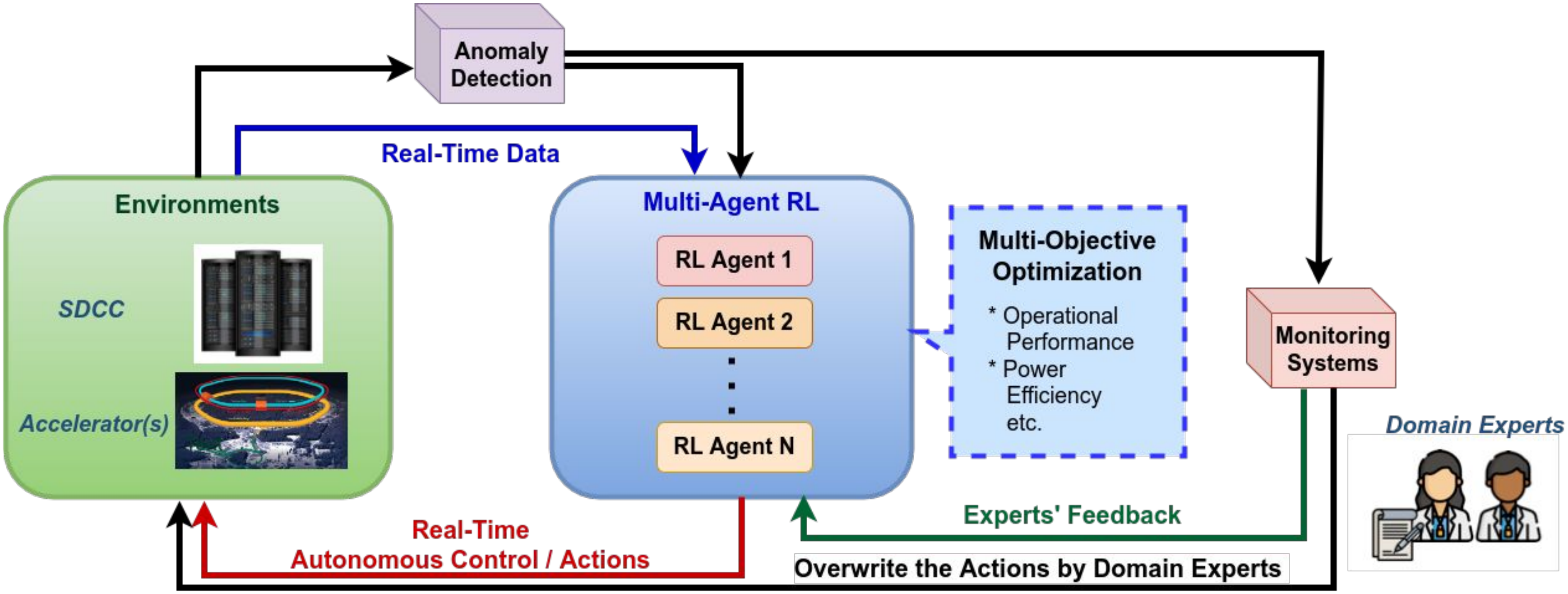
Intelligent Autonomous Control with Human-AI-Facility Integration



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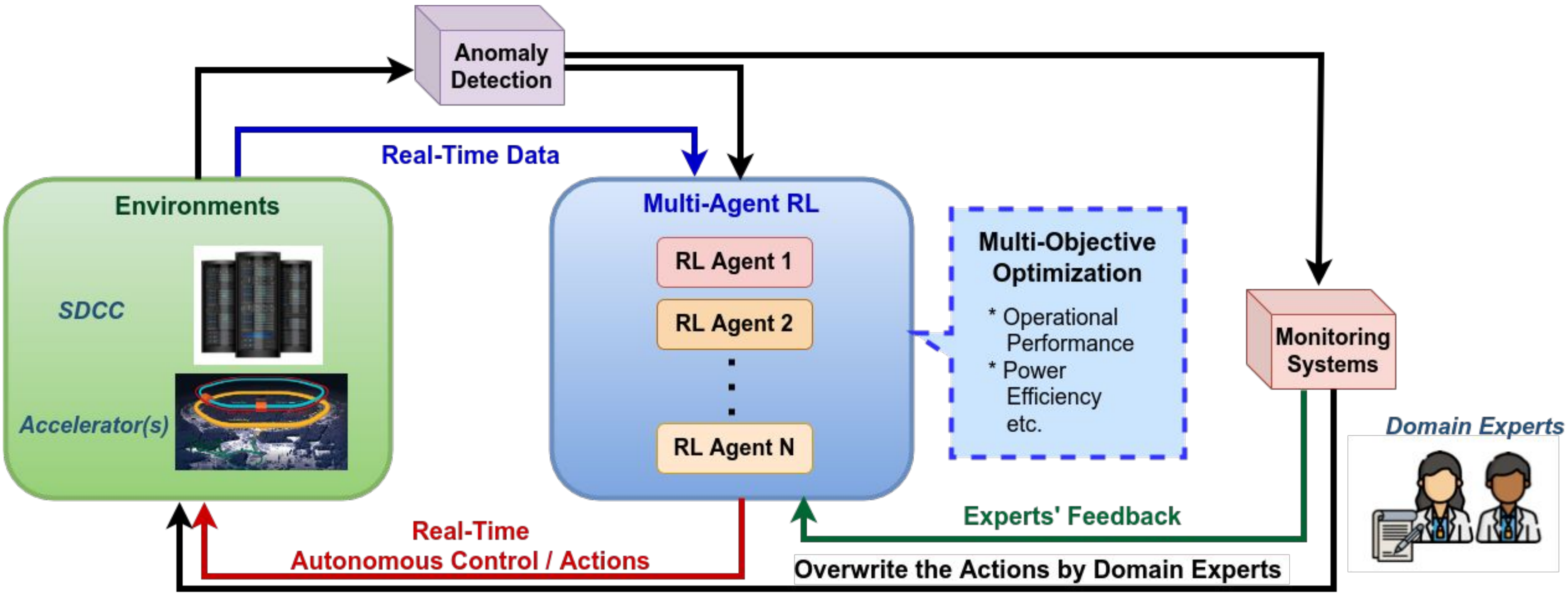
Solution: Develop a novel **multi-objective RL algorithm** to **jointly optimize multi-criteria** (i.e. operational performance and power-efficiency) for SDCC and Accelerators.

Intelligent Autonomous Control with Human-AI-Facility Integration



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