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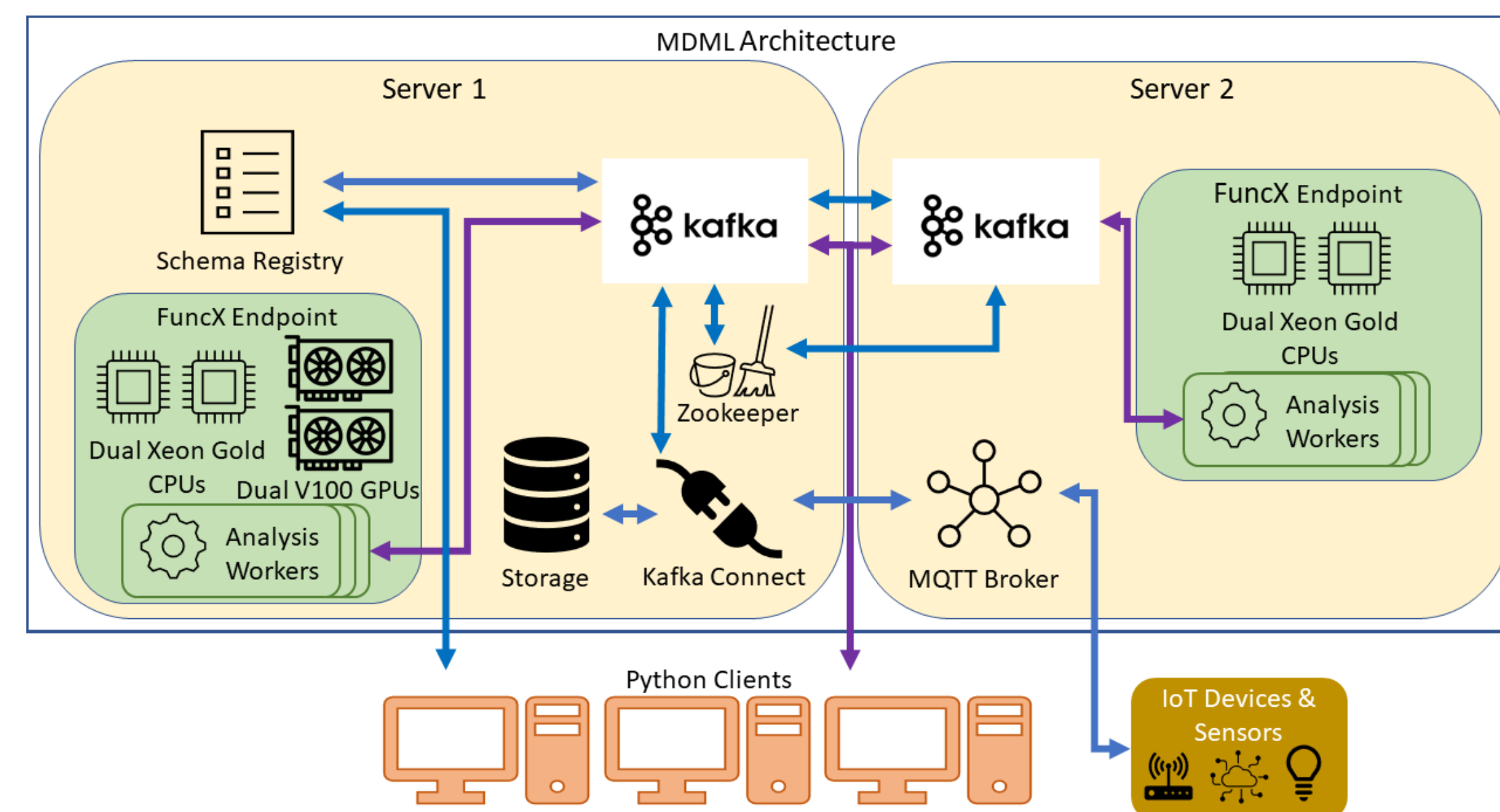
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Our (Big) Goals

- Design a software framework for *self-driving labs*
- Accelerate discovery via intelligent experimentation
- Democratize lab-work by building open-source tools

Streaming data from multiple sources

The *MDML* is a Kafka based platform for streaming, analyzing, and logging experiment and simulation data



Model-based optimization and learning

Sum-of-squared simulation outputs:

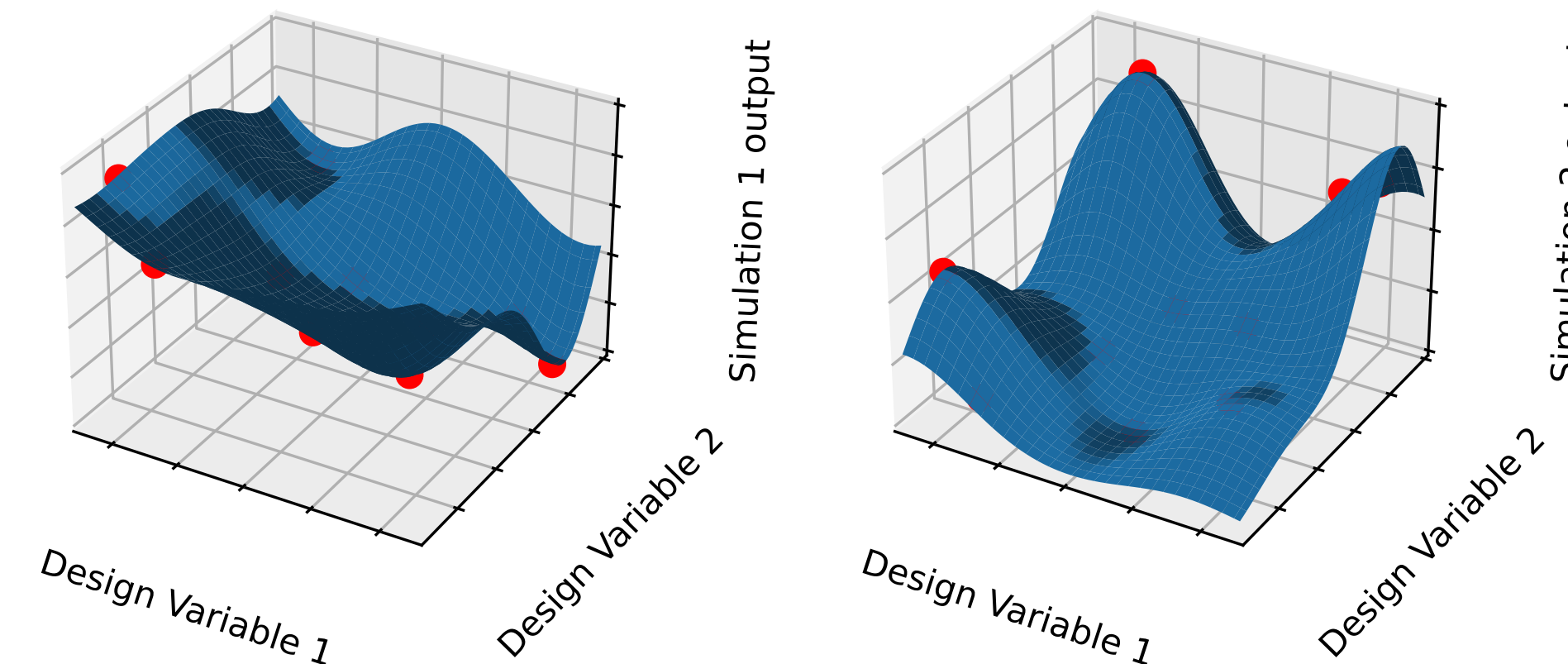
$$\min_{x \in \mathcal{X}} \left(\sum_{i=1}^{m_1} S_i(x)^2, \sum_{j=1}^{m_2} S_j(x)^2 \right)$$

One simulation, one algebraic objective:

$$\min_{x \in \mathcal{X}} \left(S(x), \sum_{i=1}^n x^2 \right)$$

Response Surface Methodology

- **Search/sample** data for raw **simulations outputs**
- Use **surrogates** to model **simulations**, **not objectives**
- Separately define **objectives and constraints**
- Scalarize **objectives** using **acquisition functions**
- **Solve scalarized surrogate problems** and iterate



Design Principles

Mix-and-match

- Initial search (design-of-experiments)
- Surrogate models
- Acquisition/scalarization functions
- Scalar optimization solvers

Easy for users and developers

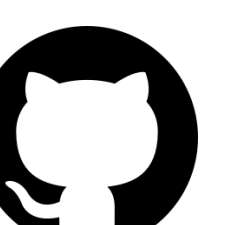
- Support for variety of design vars and simulations
- Support various scientific workflows
- Embed/extract problems from unit cube

Flexible problem definitions

- Add design vars, sims, objs, + constraints
- Add searches, surrogates, acquisitions, optimizer
- Solve serially or in parallel using `libEnsemble`

Download ParMOO

- `git clone https://github.com/parmoo/parmoo`
- `pip install parmoo`



Continuing Work

- Continue to add new solvers and techniques
- Support wider variety of problems & workflows