# A framework for fully autonomous design of materials via multiobjective optimization and active learning: challenges and next steps

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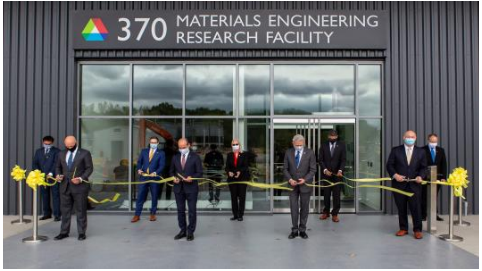
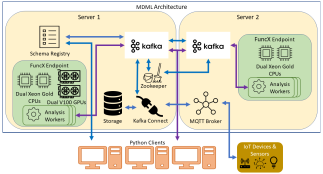
# Big Picture

The Argonne Material Engineering Research Facility (MERF):




Accelerate experimentation → production pipeline with ML:

←

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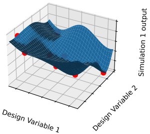
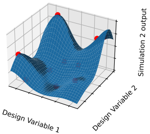


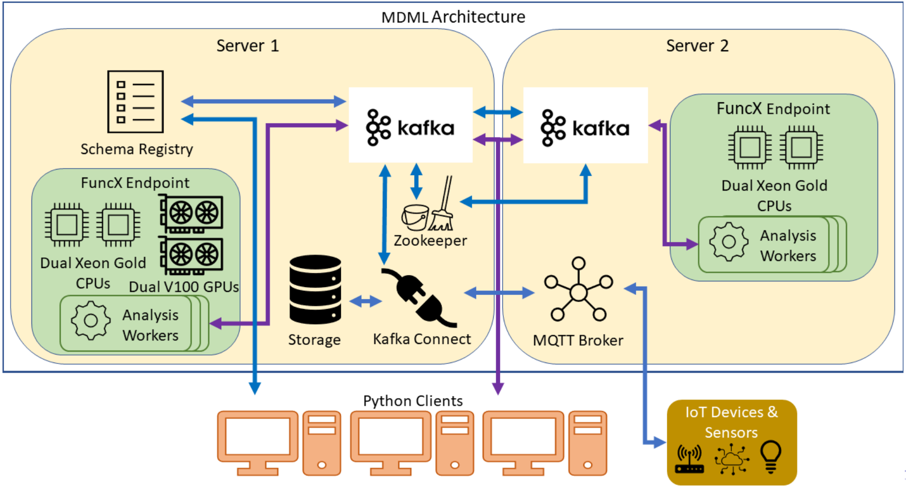



# Our (Big) Goals

- 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

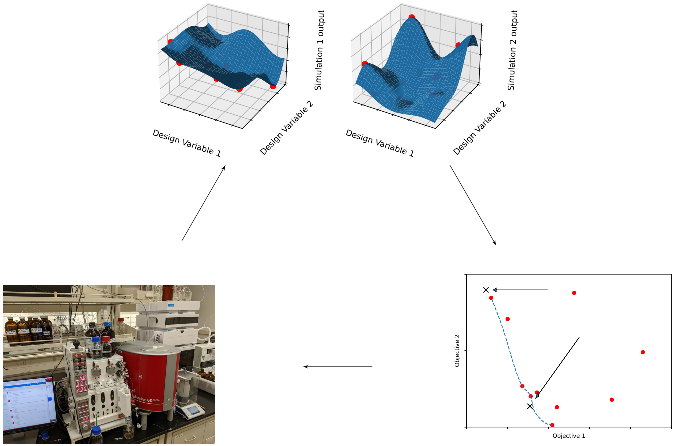
- How to collect and analyze data?
- MDML is a platform for streaming, analyzing, and logging experiment and simulation data (used at the MERF)



# Model-based optimization

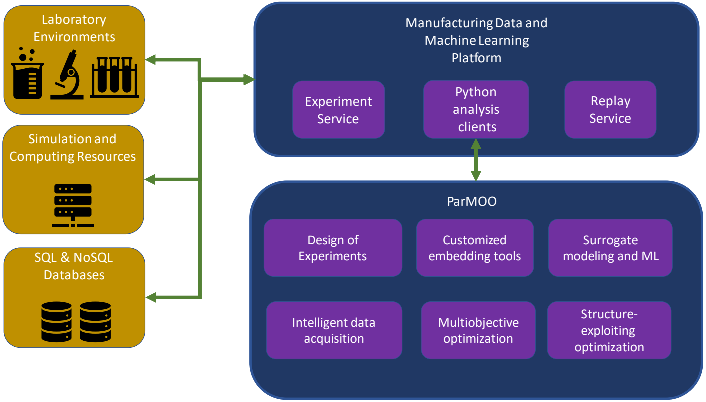
- ParMOO (multiobjective optimization) library is used to implement an active learning loop

ParMOO fits surrogate models to the experiment/simulation data



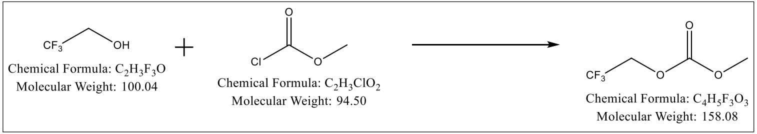
# Our framework and software stack

- MDML gives us access to *heterogeneous data from laboratory sources*
- ParMOO gives us modular/customizable *modeling, embedding, and solvers*



# Example: TFMC Manufacturing Conditions

Optimize the production of TFMC via a known reaction...




Trifluoroethanol

Methyl chloroformate

2,2,2-trifluoroethyl
Methyl carbonate

Solvent: acetonitrile

Base: N,N-Diisopropylethylamine

... in LabVIEW automated CFR
and measured via NMR

Left to right:
PC running LabVIEW
CFR and feed
NMR spectroscope

# Problem definition

- **Want to maximize TFMC production at high temperatures**
- High temperatures trigger a side-reaction and produces byproduct (TFE)
  - **Minimize TFE production**

*Design variables and bound constraints for experiment:*

| Parameter | Lower bound | Upper bound |
|---|---|---|
| Temperature (degrees C) | 40 | 150 |
| Reaction time (seconds) | 60 | 300 |
| Equivalence ratio (no units) | 0.9 | 2 |

# Challenges and Solver Settings

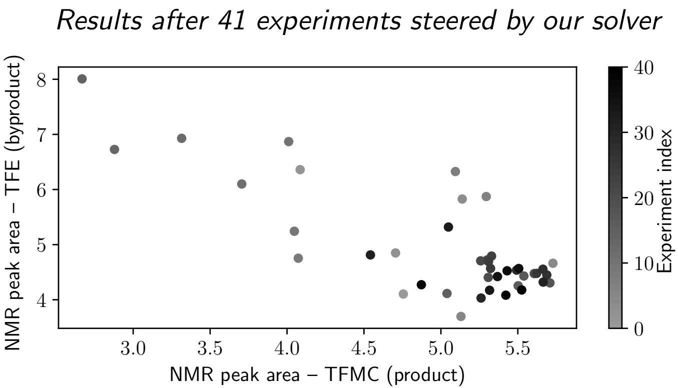
Solve a small problem on an extremely limited budget:

- 3 variable, 2 objective problem
- Experiments take about 10 mins and we have limited supply of reagent materials
- About 50 experiments max

Solver settings:

- 15-pt Latin hypercube, Gaussian RBF surrogate, L-BFGS-B optimizer
- 3 scalarizations per batch, sorted by temp (to speedup reaction)
- evaluated batch on CFR, TFMC and TFE peaks recorded by NMR

# Experiment Results

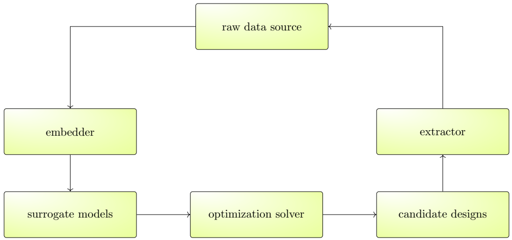


# Next Steps

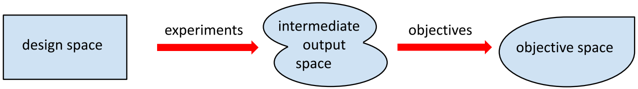
Need to handle more complex design spaces:

- Custom embeddings (including generative AI)
- Trust-region descent / subspace iterations

- Custom surrogate models
- Structure-exploiting optimizers




(Top) using custom embedders to optimize in latent space



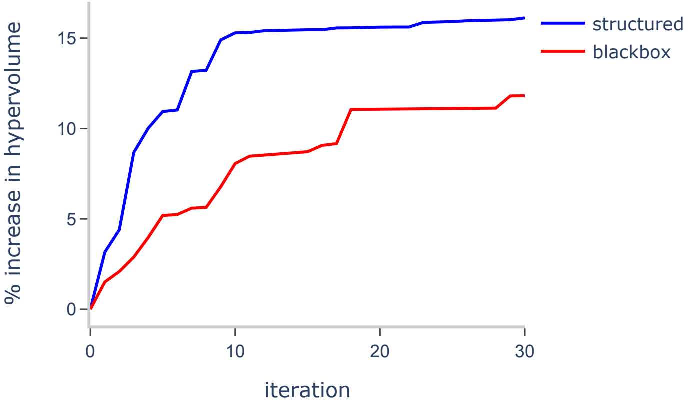

(Bottom) exploiting problem structure using composite objectives

# A sneak peek!

We created a surrogate problem based on this data to explore next steps!

`https://github.com/parmoo/parmoo-solver-farm`
$\rightarrow$ `cfr-material-design-2022`

5 variable (2 categorical), 3 objectives (1 cheap) problem



Email: `tchang@anl.gov`

We love open source!

```
git clone https://github.com/parmoo/cfr-materials
pip install REQUIREMENTS.txt
```

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