

ParMOO: A Python library for parallel multiobjective simulation optimization

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SIAM CSE 23

Outlines

Introduction to MOSO + my experience

3 challenges + solutions

ParMOO software design + release

Example Problems

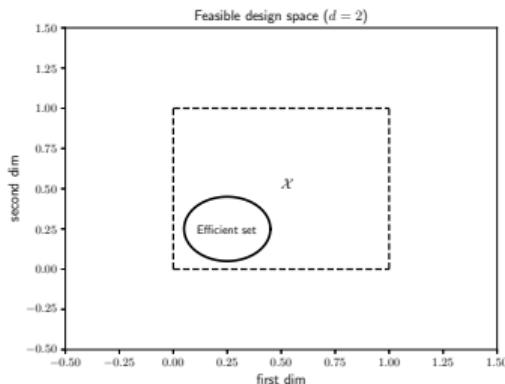
Grand challenges + some closing thoughts

Multiobjective Optimization Problems

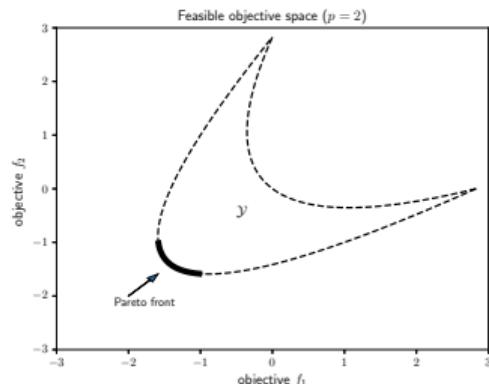
$$\min_{x \in \mathcal{X}} F(x)$$

Multiobjective Optimization Problems

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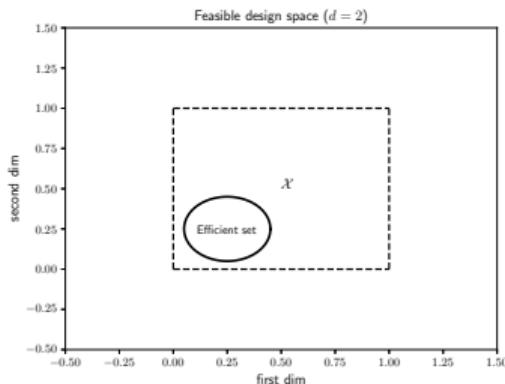


$$F : \mathcal{X} \rightarrow \mathcal{Y}$$



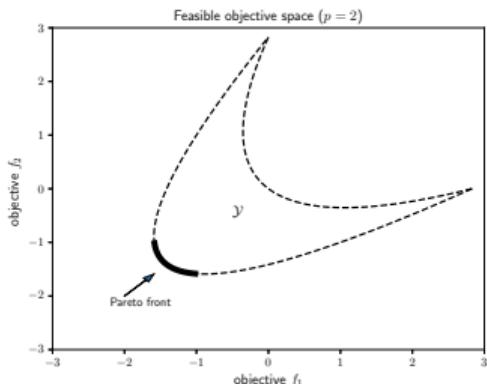
Multiobjective Optimization Problems

$$\min_{x \in \mathcal{X}} F(x)$$



$F : \mathcal{X} \rightarrow \mathcal{Y}$

expensive
blackbox process

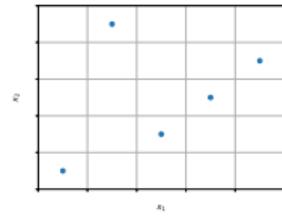


Multiobjective Response Surface Methodology

or Model-Based Optimization or Active Learning

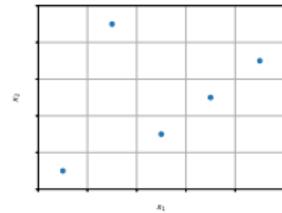
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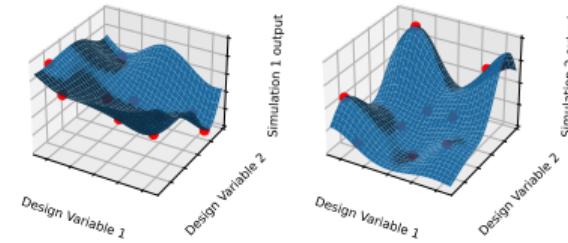
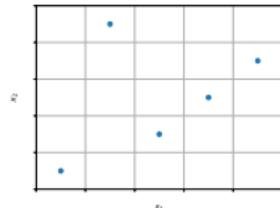
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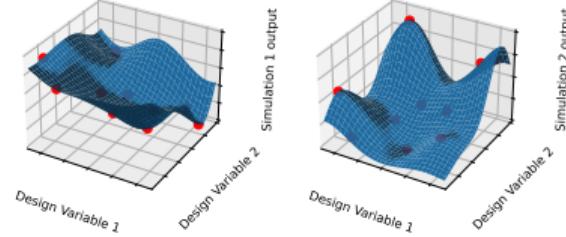
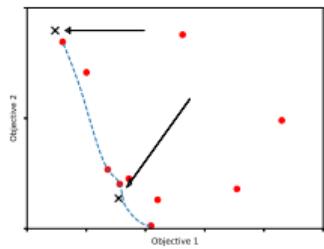
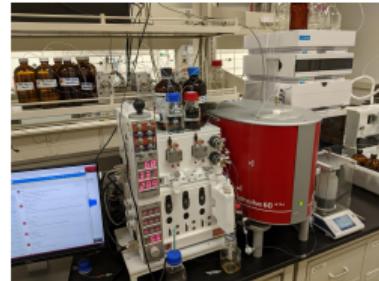
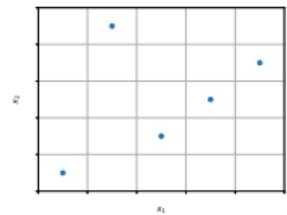
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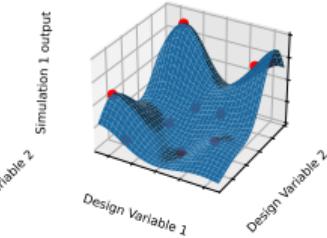
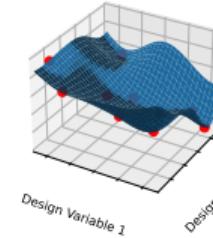
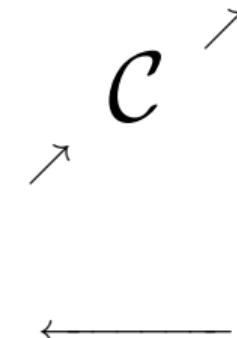
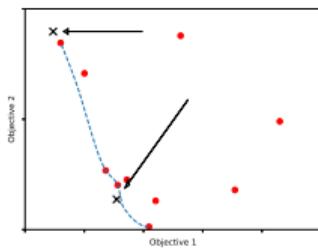
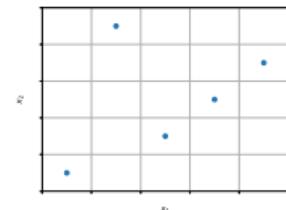
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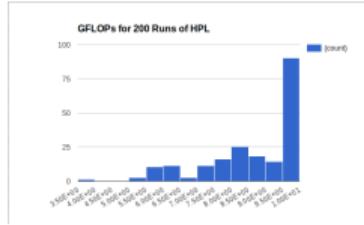


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Example: HPC Performance Tuning

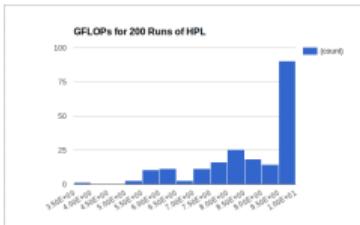


VT VarSys Project – 40 runs of HPL



ANL – LCRC Computing Resources: Bebop

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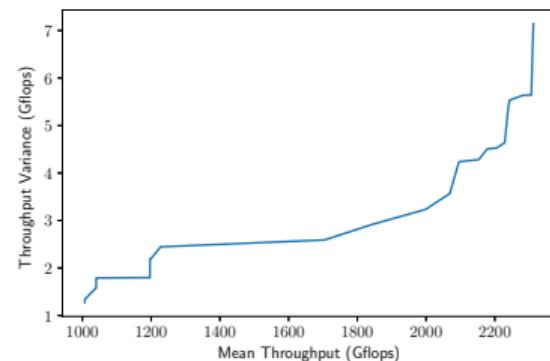


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VTMOP solver



[1] Chang et al. Multiobjective optimization of the variability of the high-performance LINPACK solver. In Proc. WSC 2020.

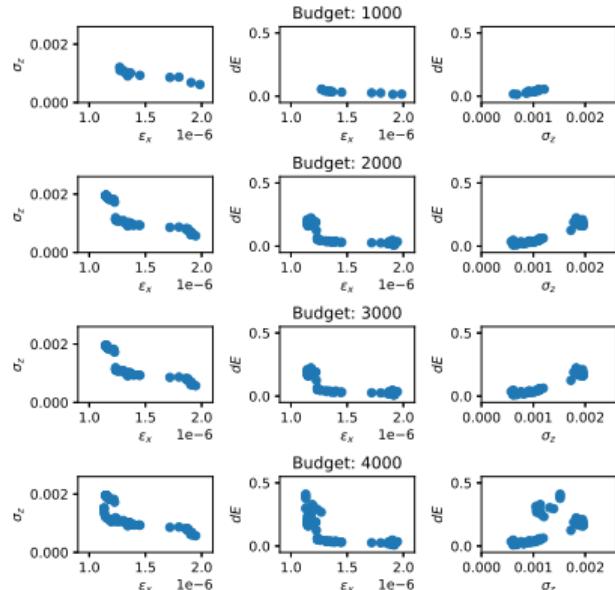
Challenge 1: **mixed vars + problem types**

Example: Particle Accelerator Design

OPAL-t
(Object Oriented Parallel
Accelerator Library for
beam-lines + linacs)

```
OPAL.dat
MUTriplet benchmark input file
Tennessee Accelerator Laboratory, University of Tennessee
10<.out>          output file name (optional)
0<.in>             device file (optional, if present, file)
4<.n>              # of problems sizes (M)
20 30 35 40         Ns
2<.m>              # of MPs
1 2 3 4             NPs
0<.p>              # of process grids P = n! / 3!
2 1 4              Ps
0<.t>              Ts
10.0               threshold
3<.r>              # of parallel fact
0 1 2               PMFACT (0=left, 1=right, 2=right)
2<.c>              # of recursive stopping criterium
0<.rec>             NCFACT
1<.r>              # of panels in recursion
0<.d>              NCFACT
3<.r>              # of recursive panel fact.
PMFACT (0=left, 1=right, 2=right)
1<.t>              TFACT
BCM3D (0=1x1,1=1x1,2=2x2,3=2x4,4=4x4,5=5x5)
1<.t>              TFACT
0<.t>              TFACT
DEPTHS (<n>)
0<.t>              TFACT
0<.t>              TFACT
0<.t>              TFACT
L1 in (0=transposed,1=same-transposed) Term
0<.t>              TFACT
0<.t>              TFACT
Equilibrium (0=none,1=real)
memory alignment in double (> 0)
```

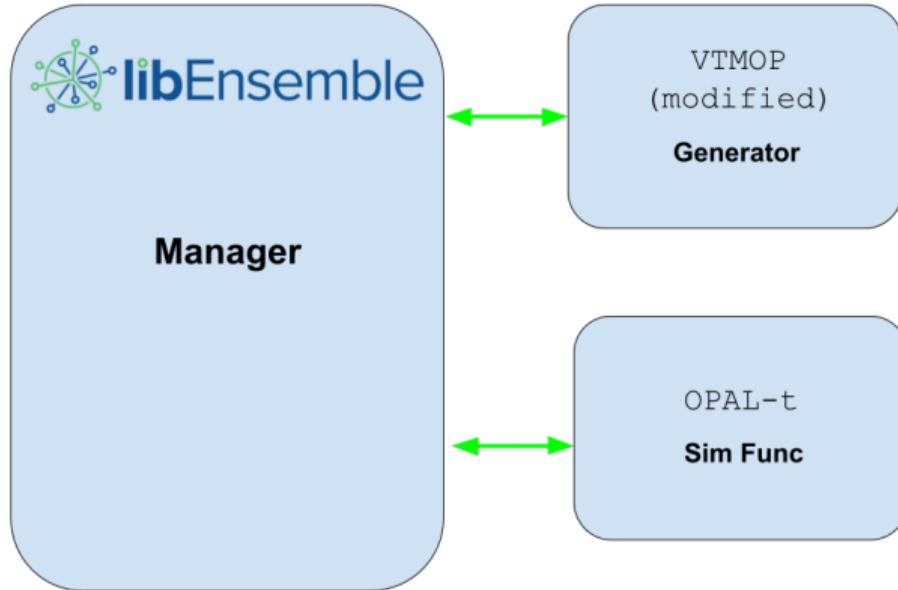
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[3] Neveu et al. Comparison of multiobjective optimization methods for the LCLS-II photoinjector. CPC 283:108566 (2023).

Handling parallel evals



[4] Chang et al. Managing computationally expensive blackbox multiobjective optimization problems with libEnsemble. In Proc. SpringSim 2020.

Challenge 2: **parallel evals + computing environments**

Commercial solutions

Commercial solutions

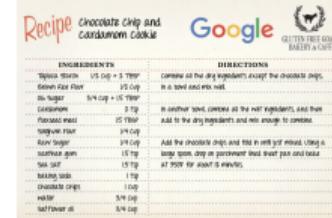


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Commercial solutions



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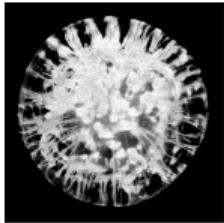


"The makings of a smart cookie" by Daniel Golovin on Google Research Blog.

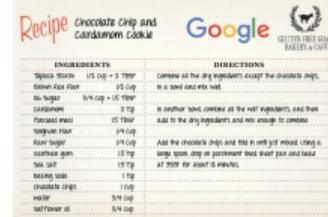
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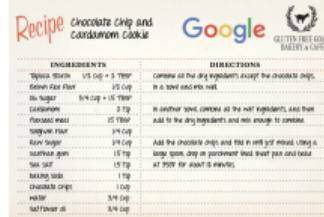


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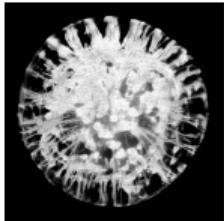
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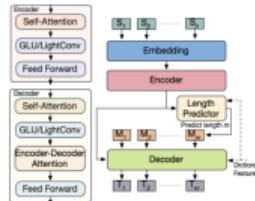
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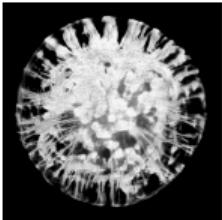


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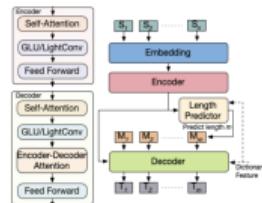
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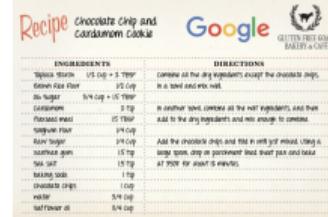
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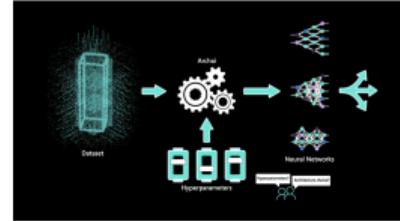
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"Archai can design your neural network with state-of-the-art NAS" by Shital Shah et al. on Microsoft Research Blog.

Commercial solvers

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General purpose: (solver + backend)

Google – OSS Vizier + Pythia backend

[5] Song et al. *OSS Vizier: distributed infrastructure and API for reliable and flexible black-box optimization*. In Proc. 2022 AutoML-Conf.

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Special purpose: (solver + special purpose deployment)

IBM – Querry-based Molecular Optimization (QMO)

[7] Hoffman et al. *Optimizing molecules using efficient queries from property evaluations*. Nature Machine Intelligence 4:21–31 (2022).

Microsoft – Archai for NAS

[8] Shah et al. *Archai: platform for neural architecture search*. Microsoft Research (Jul, 2022).

SOA in structure-exploiting blackbox optimization

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"Optimization and root finding (scipy.optimize)" in SciPy v1.10.0 [9].

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SOA in structure-exploiting blackbox optimization



SciPy

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Stochastic dimension reduction explained in this context by Stefan [10].

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SOS structure can be exploited by DFO solver POUNDERS in TAO [11].

[9] Virtanen et al. SciPy 1.0: fundamental algorithms for scientific computing in Python. *Nature Methods* 17:261–272 (2020).

[10] Wild. Optimization and learning with zeroth-order stochastic oracles. *SIAM News* 56(1):1,3 (2023).

[11] Wild. Solving derivative-free nonlinear least squares problems with POUNDERS. *Adv. and Trends in Optimization with Engineering Applications*, Ch. 40, pp. 529–540 (2017).

Challenge 3:

SOA optimization + exploiting problem structure

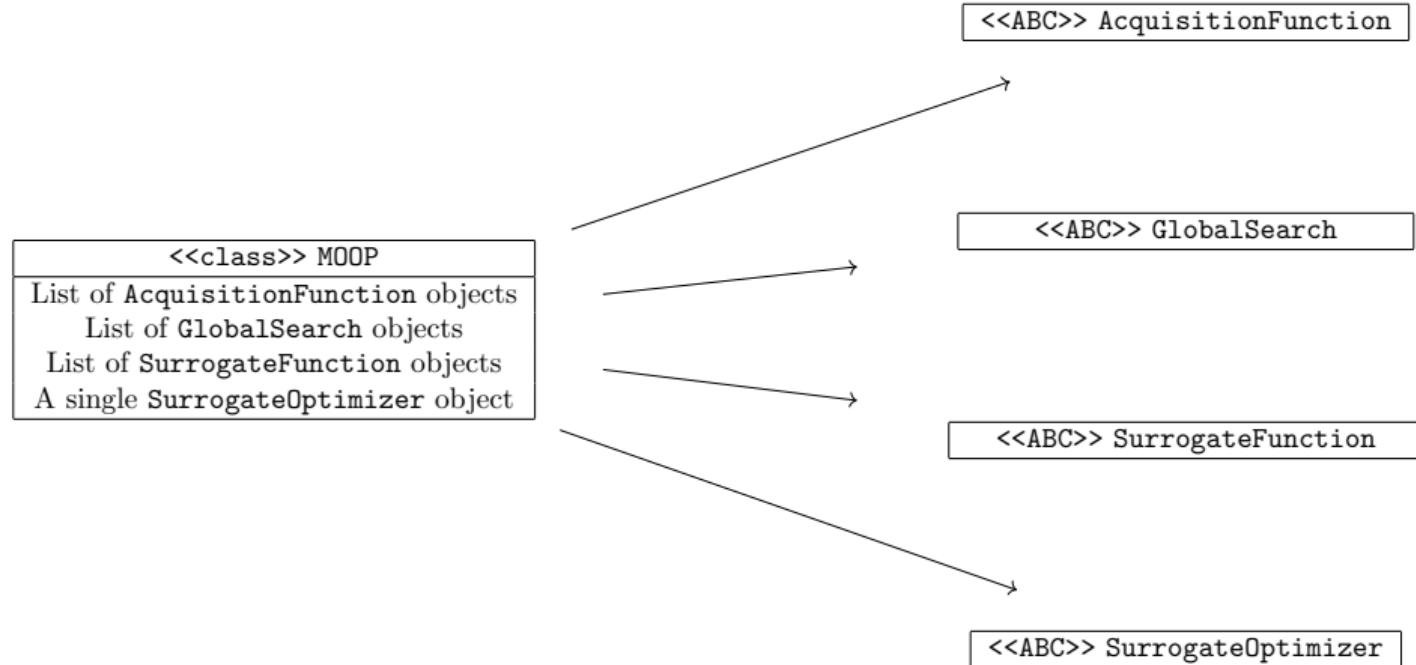
Design goals:

1. Highly customizable framework for multiobjective RSM
2. Flexible problem types (mixed-variables, constraints, etc.)
3. Easy to use, deploy, and extend (unforeseen use-cases and environments)
4. Solve large-scale problems + exploit structure and domain knowledge

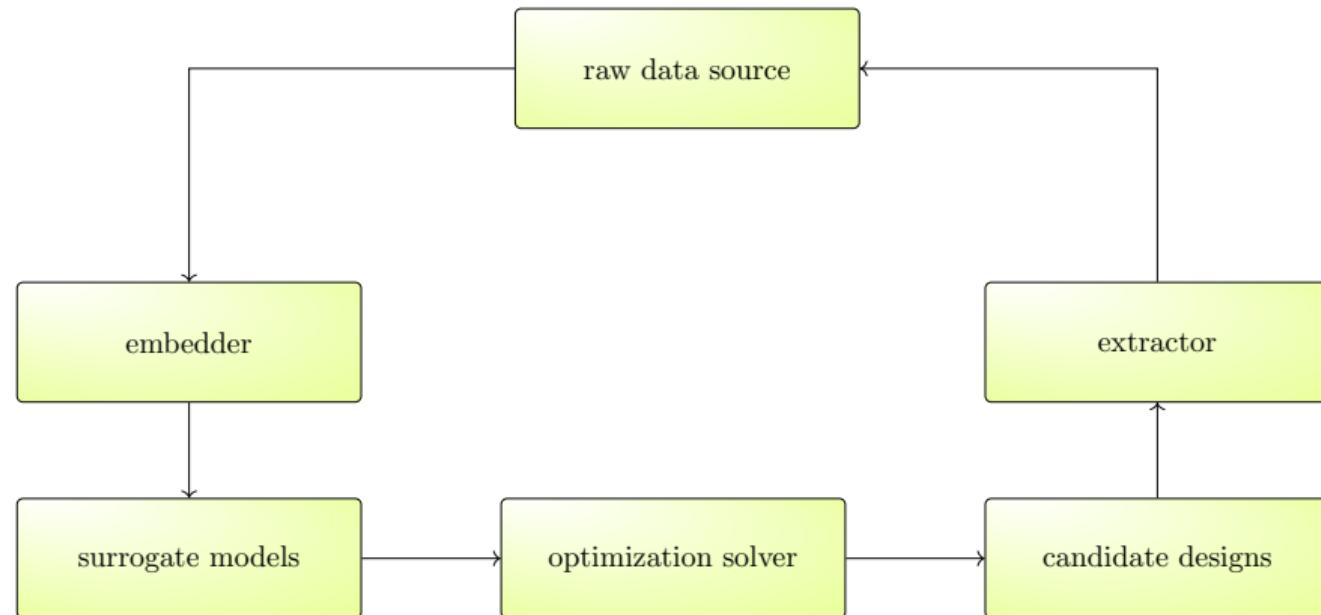
[12] Chang and Wild. *Designing a framework for solving multiobjective simulation optimization problems*. In prep.

Goal 1: Customizability

ParMOO UML:



Goal 2: Flexible problem types



Goal 3: Easy to deploy

Extend MOOP base class and overwrite MOOP.evaluateSimulation() evaluator backend.

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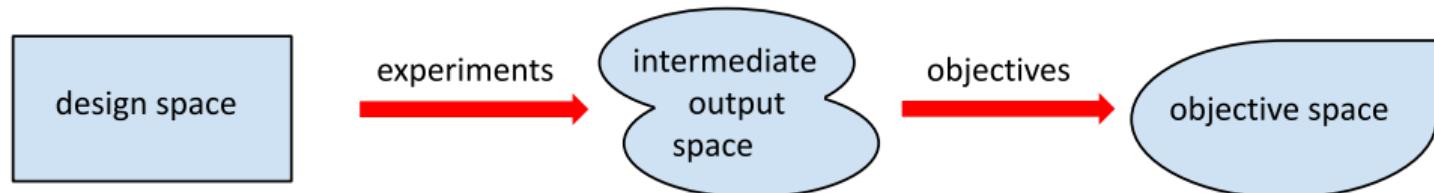
Examples:

- ▶ parallel simulation evaluations on HPC systems with libEnsemble [13]
- ▶ streaming experiment data via Kafka producer/consumer requests with the MDML [14]

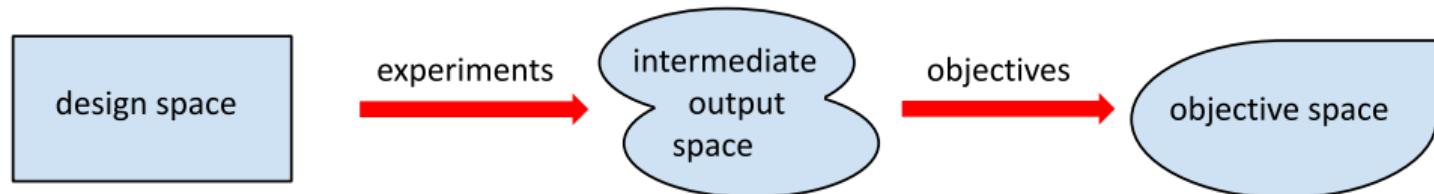
[13] Hudson et al. *libEnsemble: a library to coordinate the concurrent evaluation of dynamic ensembles of calculations*. IEEE TPDS 33(4):977–988 (2021).

[14] Elias et al. *The manufacturing data and machine learning platform: enabling real-time monitoring and control of scientific experiments via IoT*. In Proc. 2020 IEEE WF-IoT.

Goal 4: problem structure



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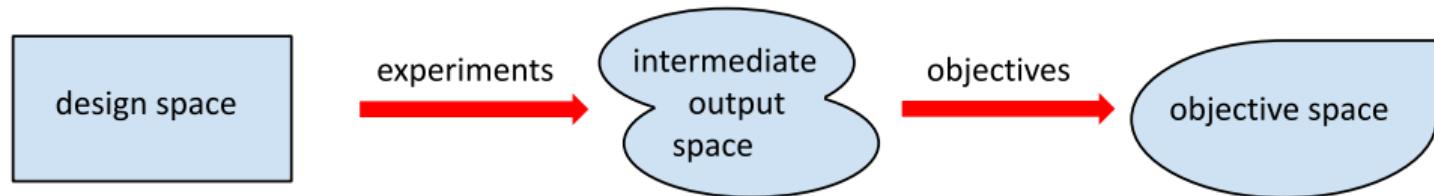
Sum-of-squares structure:

$$h_i(x, S(x)) = \sum_{j \in N_i} (S_j(x))^2$$

where each N_1, \dots, N_o is an index set.

Increases order of approximation \Rightarrow
increases order of convergence

Goal 4: problem structure



Sum-of-squares structure:

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Increases order of approximation \Rightarrow
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Heterogeneous MOOPs:

$$\begin{aligned} h_1(x, S(x)) &= S_1(x) \\ h_2(x, S(x)) &= \|x\|^2 \end{aligned}$$

Use expensive surrogate models for h_1 (i.e., S_1) but not for h_2

Sample code

```
from parmoo import MOOP
from parmoo.optimizers import LocalGPS as gps
from parmoo.searches import LatinHypercube as lhs
from parmoo.surrogates import GaussRBF as rbf
from parmoo.acquisitions import UniformWeights as wsum
# Create MOOP object with GPS optimizer
moop = MOOP(gps)
# Add a continuous + categorical design variable
moop.addDesign({'name': "x1", 'lb': 0.0, 'ub': 1.0})
moop.addDesign({'name': "x2", 'des_type': "cat", 'levels': 3})
# Define and add a simulation function (with surrogates and search)
def s(x): return [(x["x1"]-.2)**2, (x["x1"]-.8)**2] if x["x2"]==0 else [9,9]
moop.addSimulation({'name': "sim", 'm': 2, 'sim_func': s,
                     'search': lhs, 'surrogate': rbf})
# Add 2 objectives
moop.addObjective({'name': "f1", 'obj_func': lambda x, s: s["sim"][0]})
moop.addObjective({'name': "f2", 'obj_func': lambda x, s: s["sim"][1]})
# Add 3 weighted-sum acquisition functions
for i in range(3):
    moop.addAcquisition({'acquisition': wsum})
# Solve with 5 iterations and fetch numpy struct of solutions
moop.solve(5)
results = moop.getPF()
```

ParMOO Release



Written in Python

Version 0.2.0 is now available on pip,
conda-forge, and GitHub



<https://github.com/parmoo/parmoo>



<https://parmoo.readthedocs.io>

[15] Chang and Wild. ParMOO: A Python library for parallel multiobjective simulation optimization. *JOSS* 8(82):4468 (2023).

Example 1: Fayans EDF Model Calibration

Find params $x \in [0, 1]^{13}$ to fit the Fayans model to data d_i :

$$M(\xi_i; x) \approx d_i \quad i = 1, \dots, 198$$

ParMOO simulation:

$$S_i(x) = M(\xi_i; x) - d_i, \quad i = 1, \dots, 198;$$

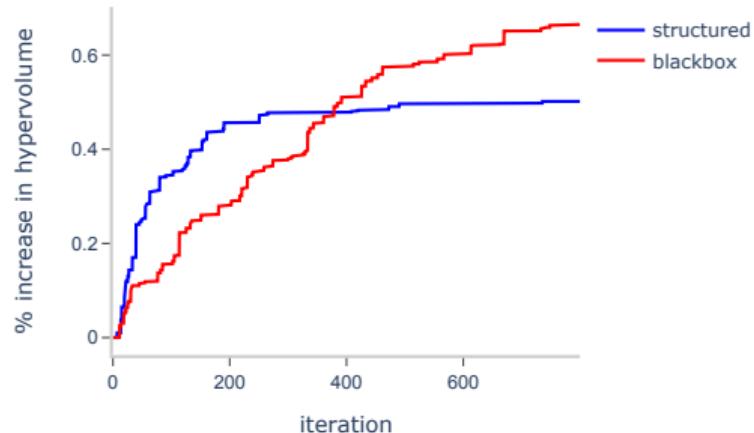
Min SOS across 3 observable classes

$$F_t = \sum_{i=1}^{m_t} (S_{t,i}(x))^2$$

[16] Bollapragada et al. Optimization and supervised machine learning methods for fitting numerical physics models without derivatives. *Journal of Physics G: Nuclear and Particle Physics* 48(2):024001 (2020).

Fayans Solution with ParMOO

- ▶ Approximated Fayans model using inv dist weighting on existing dataset
- ▶ Implemented parallel solver in ParMOO using libEnsemble
- ▶ Just **14-25 lines of Python code**
- ▶ Ran for **10K** sim evals
- ▶ Compared against **same solver w/o exploiting SOS structure**
- ▶ Structure-exploiting is better at small budgets, blackbox can be better at large budgets



Example 2: Material Manufacturing with ParMOO

Choose optimal settings for material manufacturing in a continuous flow reactor (CFR)

We know how to make a desired material, need to produce at scale:

1. **Maximize the product** (battery electrolyte: TFML)
2. Can increase temperature to **reduce reaction time**
3. Too much heat activates a side reaction; need to **minimize unwanted byproduct**

Challenges:

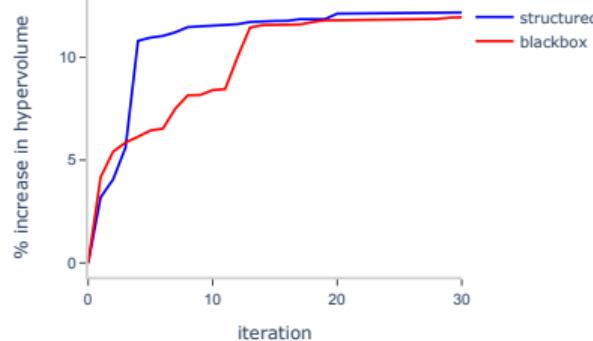
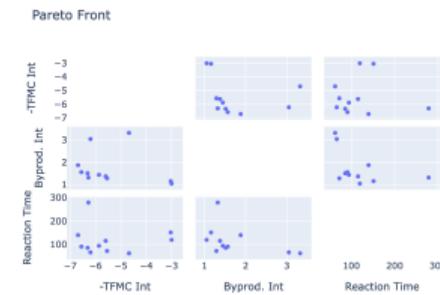
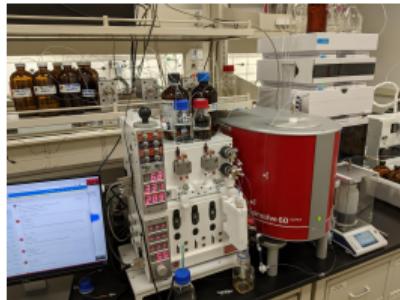
- ▶ Mixed variable types
- ▶ Heterogeneous objectives
- ▶ Must send experiments to run on CFR

CFR Optimization with ParMOO

Extend MOOP class to send/receive experiment data using MDML library (Apache Kafka)

Used categorical variable embeddings

Modeled Product/Byproduct as simulations and reaction time using algebraic equation of input



[17] Chang et al. A framework for fully autonomous design of materials via multiobjective optimization and active learning: challenges and next steps. Under review.

Grand Challenges

References

- [1] Chang et al. Multiobjective optimization of the variability of the high-performance LINPACK solver. In Proc. WSC 2020.
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Resources

GitHub: github.com/parmoo/parmoo

Docs: parmoo.readthedocs.io

PyPI: pip install parmoo

Conda: conda install --channel=conda-forge parmoo

E-mail: tchang@anl.gov

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