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

Conclusions + some closing thoughts

Multiobjective Optimization Problems

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

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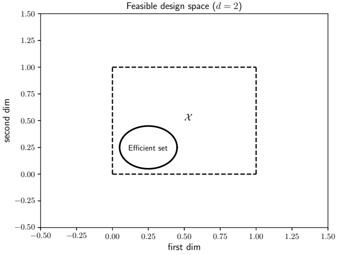
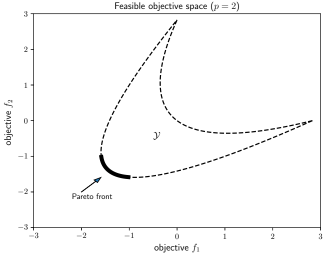


$$\longrightarrow$$

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



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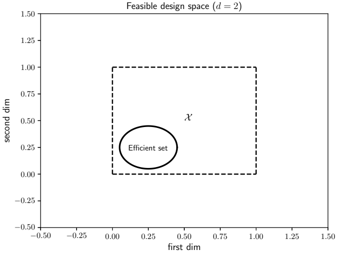

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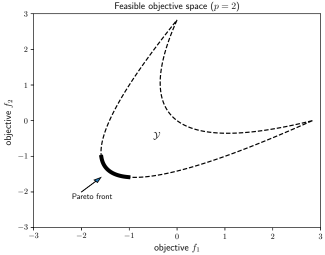
$$F : \mathcal{X} \to \mathcal{Y}$$

expensive
blackbox process



Multiobjective Response Surface Methodology

or Model-Based Optimization or Active Learning

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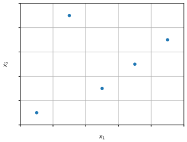

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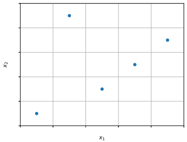

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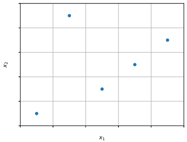

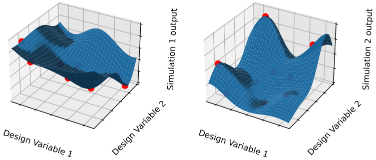

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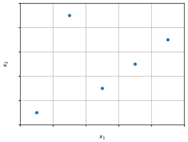

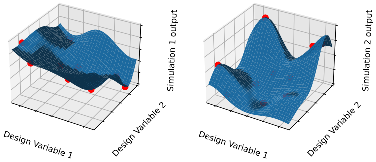

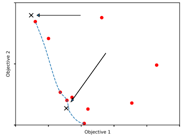

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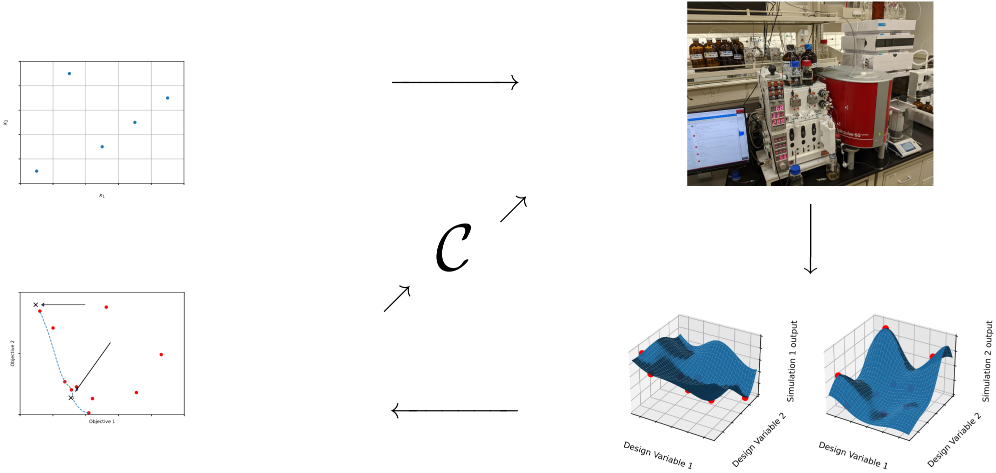
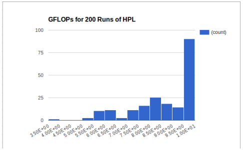


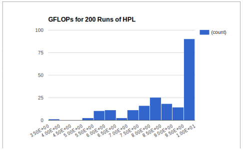
Example: HPC Performance Tuning



VT VarSys Project – 40 runs of HPL

ANL – LCRC Computing Resources: Bebop

Example: HPC Performance Tuning



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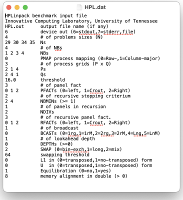
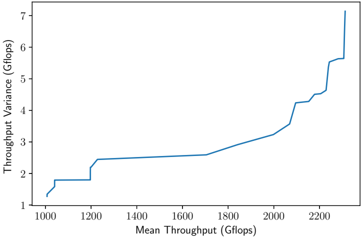



```
HPLinpack benchmark input file
Innovative Computing Laboratory, University of Tennessee
HPL.out      output file name (if any)
6            device out (6=stdout,7=stderr,file)
4            # of problems sizes (N)
29 30 34 35  Ns
4            # of NBs
1 2 3 4      NBs
0            PMAP process mapping (0=Row-,1=Column-major)
3            # of process grids (P x Q)
2 1 4        Ps
2 4 1        Qs
16.0         threshold
3            # of panel fact
0 1 2        PFACTs (0=left, 1=Crout, 2=Right)
2            # of recursive stopping criterium
2 4          NBMINs (>= 1)
1            # of panels in recursion
2            NDIVs
3            # of recursive panel fact.
0 1 2        RFACTs (0=left, 1=Crout, 2=Right)
1            # of broadcast
0            BCASTs (0=1rg,1=1rM,2=2rg,3=2rM,4=Lng,5=LnM)
1            # of lookahead depth
0            DEPTHs (>=0)
2            SWAP (0=bin-exch,1=long,2=mix)
64           swapping threshold
0            L1 in (0=transposed,1=no-transposed) form
0            U  in (0=transposed,1=no-transposed) form
1            Equilibration (0=no,1=yes)
8            memory alignment in double (> 0)
```

VTMOP solver

$\longrightarrow$



[1] Chang, Larson, and Watson. 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

Example: Parallel Runs

Challenge 2:

parallel evals + computing environments

ParMOO Design Criteria

Design goals:

1. Highly customizable framework for multiobjective RSM
2. Exploit structure and domain knowledge simulation-based optimization problems
3. Flexible problem types (mixed-variables, constraints, etc.)

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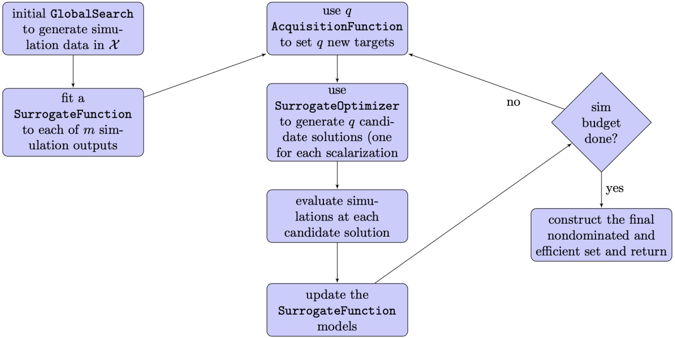
Design constraints:

1. Easy to deploy (parallelism, checkpointing, logging, flexibility)
2. Easy to maintain and extend
3. Easy to use (clean interfaces)

Customizability

ParMOO uses an object-oriented framework:



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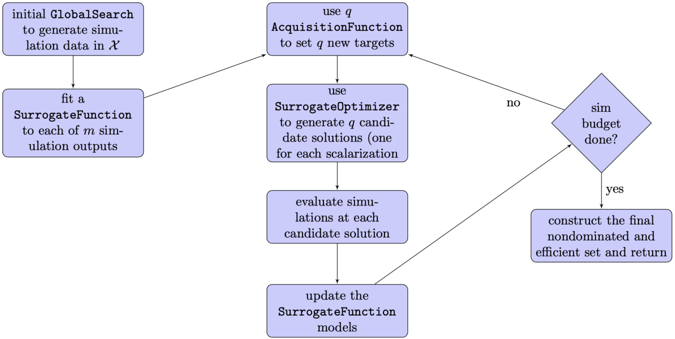
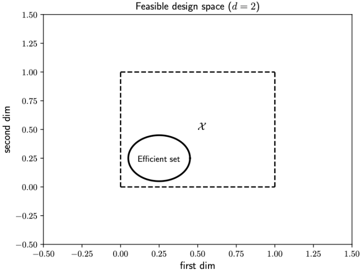


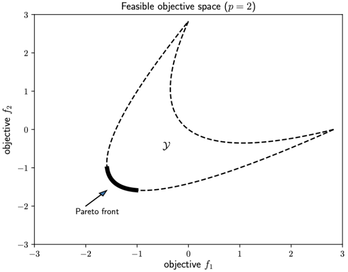
- Search/DOE
- Surrogate model
- Acquisition function
- Single-obj solver

Simulation Structure



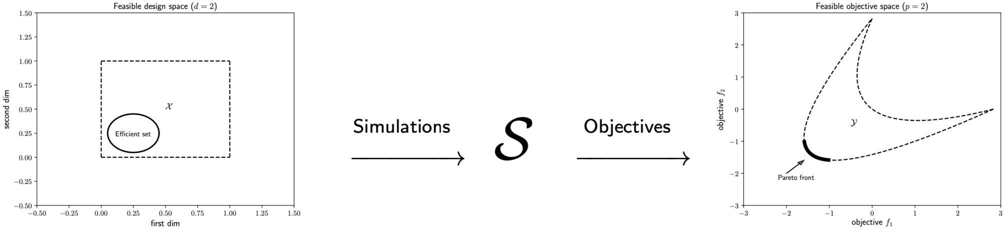
Design space

Objective Functions



Objective space

Simulation Structure



Design space *Objective space*

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where each $N_1, \ldots, N_o$ is an index set.

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Heterogeneous MOOPs:

$$h_1(x, S(x)) = S_1(x)$$
$$h_2(x, S(x)) = \|x\|^2$$

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

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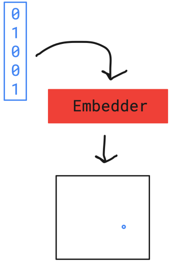

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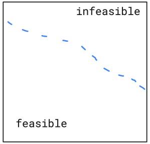

- (Nonlinear) constraints
  - Focus on *augmented Lagrangian* penalties (relax to augmented unconstrained problem)

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Easy to maintain and extend:

- OOP + total modularity makes adding new features easy
- Agile development with continuous integration
- Well-documented interface, contributing, and release process

ParMOO Release

parMOO

Written in `Python` (available on `pip` and `GitHub`)

`https://parmoo.readthedocs.io/en/latest/quickstart.html`

Combine with `libEnsemble` to use parallel solvers

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:

$$M(\xi_i; x) \approx d_i \qquad i = 1, \ldots, 198$$

ParMOO simulation:

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

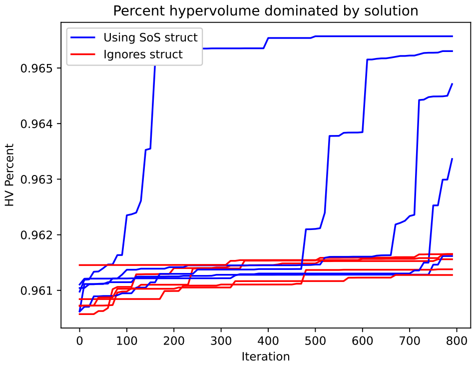
Min SOS across 3 observable classes

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

Bollapragada et al. Journal of Physics G: Nuclear and Particle Physics 48(2), 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



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:

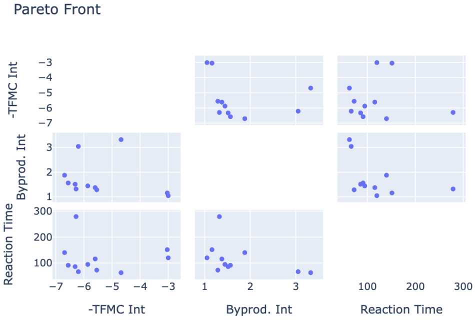
1. **Maximize the product** (battery electrolyte: TFML)
2. Can increase temperature to **reduce reaction time**
3. Too much heat activates a side reaction; need to **minimize unwanted byproduct**

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



Next Release

Coming in v. 0.2

- Interactive post-run visualization tools
- Support for customized embeddings and passing raw (unscaled) inputs
- MDML (Apache Kafka) interface for distributing simulation evalutations
- (Maybe) advanced techniques for design-of-experiments

Resources

E-mail: tchang@anl.gov
E-mail: parmoo@mcs.anl.gov

JOSS 8(82):4468 (2023)

GitHub: github.com/parmoo/parmoo
Docs: parmoo.readthedocs.io
PyPI: pip install parmoo

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