

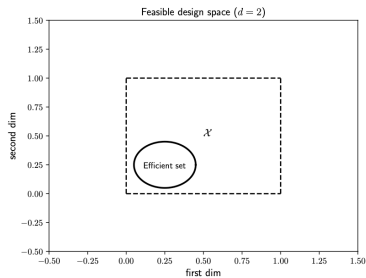
# ParMOO: A Python library for parallel multiobjective simulation optimization

Tyler Chang<sup>a</sup> and Stefan Wild<sup>a</sup>

<sup>a</sup>Mathematics and Computer Science Division,  
Argonne National Laboratory

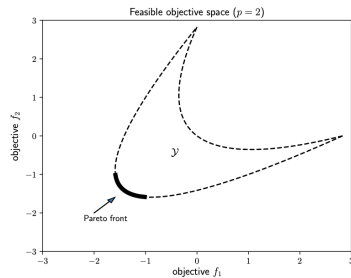
FASTMath AHM 2022

# Multiobjective \*Simulation\* Optimization



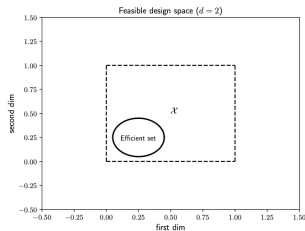
*Design space*

Objective Functions



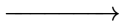
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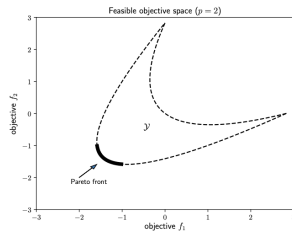
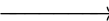
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Simulations



$\mathcal{S}$

Objectives



*Objective space*

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where each  $N_1, \dots, N_o$  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  $h_2$

## 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

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

## 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**

**Product** and **byproduct** are the result of expensive experiment,  
**reaction time** is a controllable input





E-mail: `tchang@anl.gov`

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

ParMOO is under review with JOSS

GitHub: `github.com/parmoo/parmoo`

Docs: `parmoo.readthedocs.io`

PyPI: `pip install parmoo`

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

This material is based upon work supported by the U.S. Department of Energy, Office of Science, Office of Advanced Scientific Computing Research, SciDAC program under contract number DE-AC02-06CH11357.