ParMOO: A Python library for parallel multiobjective simulation optimization

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Lawrence Berkeley National Laboratory

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

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

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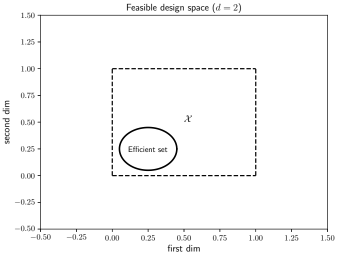
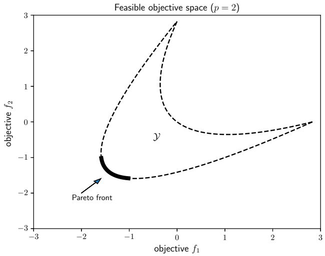


$$\longrightarrow$$

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



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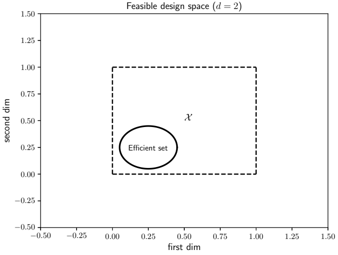
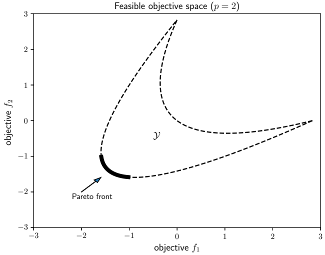


$F : \mathcal{X} \to \mathcal{Y}$

expensive
blackbox process



Multiobjective Response Surface Methodology

or Model-Based Optimization or Active Learning

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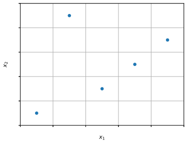

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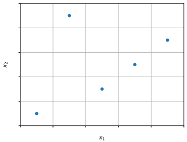

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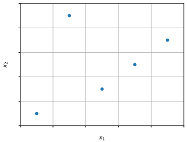

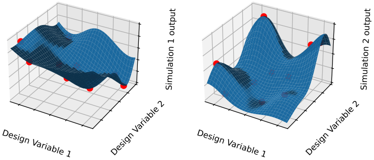

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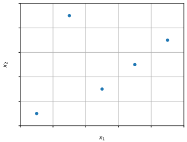

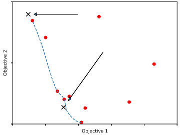

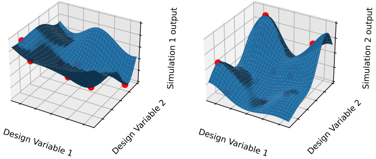

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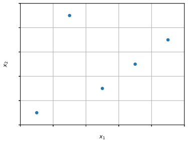
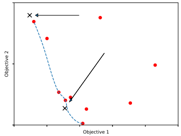
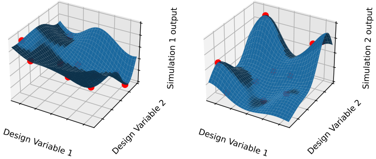
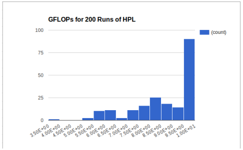


$\mathcal{C}$





Example: HPC Performance Tuning



VT VarSys Project – 40 runs of HPL

ANL – LCRC Computing Resources: Bebop

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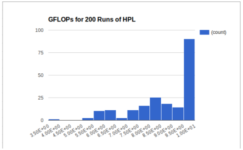

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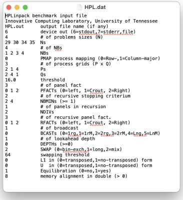
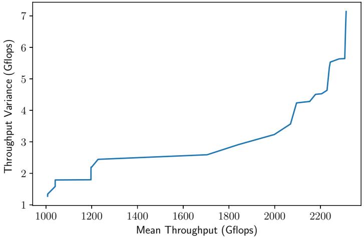


```
HPL.dat
HPLinpack benchmark input file
Innovative Computing Laboratory, University of Tennessee
HPL.out      output file name (if any)
6            device out (6=stdout,7=stderr,file)
4            # of problems sizes (N)
29 30 34 35  Ns
4            # of NBs
1 2 3 4      NBs
0            PMAP process 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

$\longrightarrow$



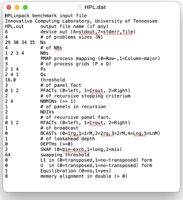
[1] Chang et al. Multiobjective optimization of the variability of the high-performance LINPACK solver. In Proc. WSC 2020.

Challenge 1:

mixed vars + problem types

Example: Particle Accelerator Design

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



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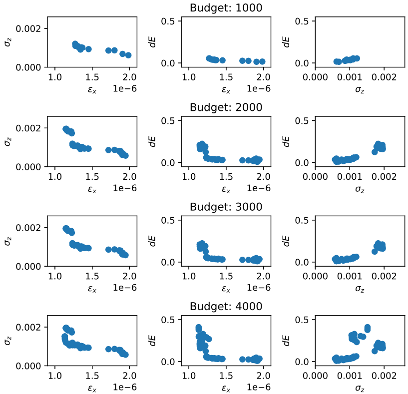
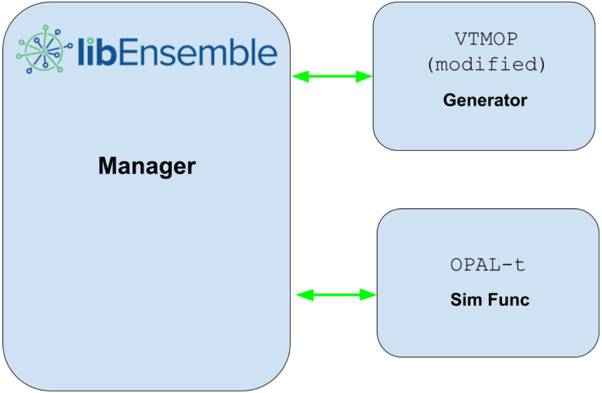
VTMOP solver



[2] Chang et al. *Algorithm 1028: VTMOP: Solver for blackbox multiobjective optimization problems. ACM TOMS 48(3):36 (2022).*

[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

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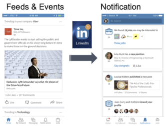

"Using Bayesian optimization for balancing metrics in recommendation systems" by Yunbao Ouyang et al. on LinkedIn Engineering Blog.

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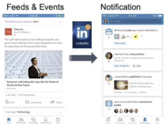

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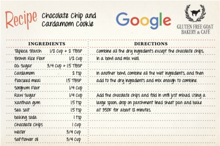

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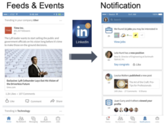

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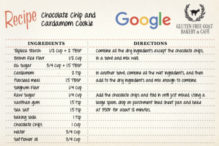

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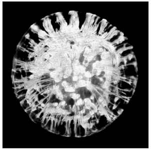

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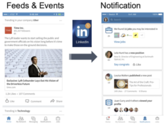

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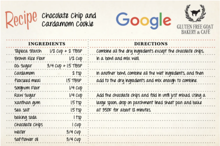

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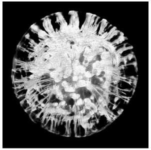

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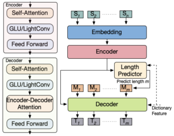

“Optimizing model accuracy and latency using Bayesian multi-objective NAS” by David Eriksson et al. on Meta Research Blog.

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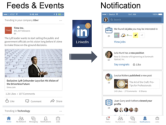

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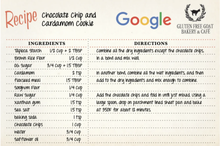

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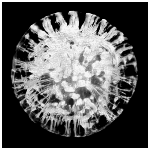

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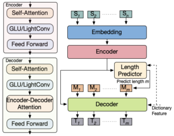

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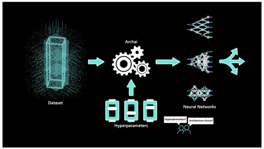

"Archai can design your neural network with state-of-the-art NAS" by Shital Shah et al. on Microsoft Research Blog.

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.

Meta – BoTorch + Ax backend

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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 and structure-exploiting blackbox optimization

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SciPy

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

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

SOA and structure-exploiting blackbox optimization

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siam news

Optimization and Learning with Zeroth-order Stochastic Oracles

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

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

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TAO

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

ParMOO Design Criteria

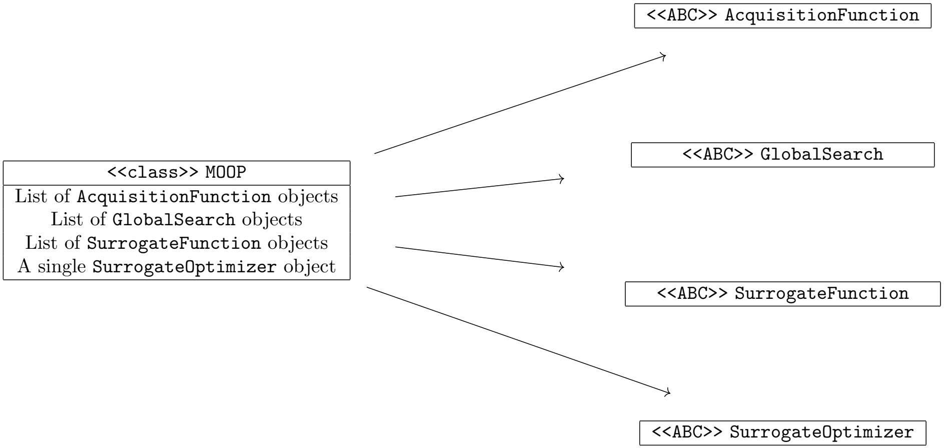
Design goals:

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

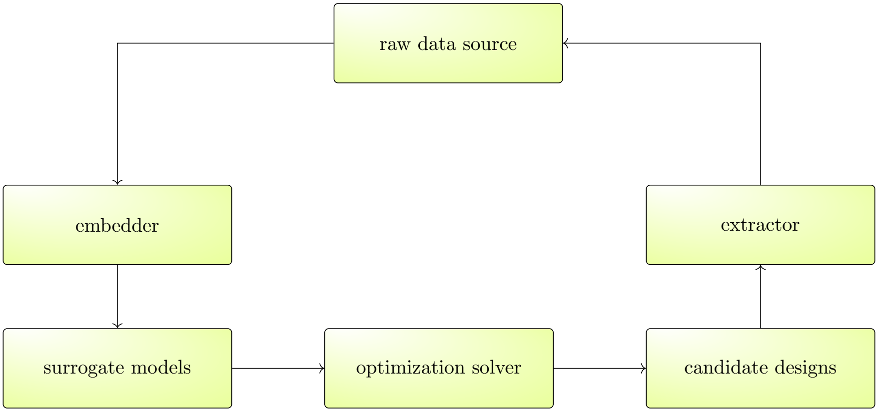
[12] Chang and Wild. Designing a framework for solving multiobjective simulation optimization problems. In prep.

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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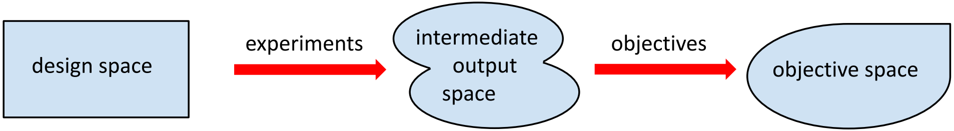
Examples:

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

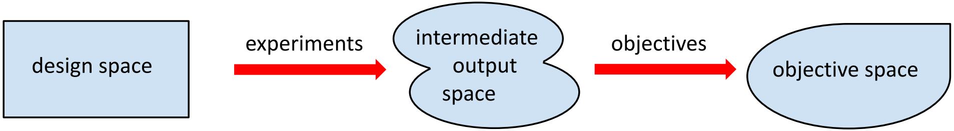
[13] Hudson et al. libEnsemble: a library to coordinate the concurrent evaluation of dynamic ensembles of calculations. IEEE TPDS 33(4):977–988 (2021).

[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



Goal 4: problem structure



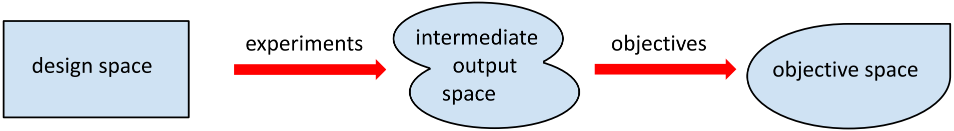
Sum-of-squares structure:

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

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

Increases order of approximation $\Rightarrow$ increases order of convergence

Goal 4: problem structure



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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

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 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:

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

ParMOO simulation:

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

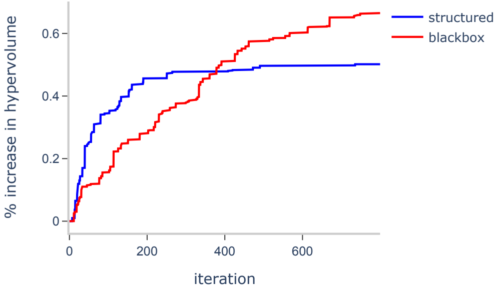
Min SOS across 3 observable classes

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

[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:

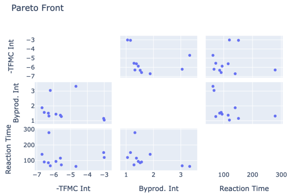
- Mixed variable types
- Heterogeneous objectives
- Must send experiments to run on CFR

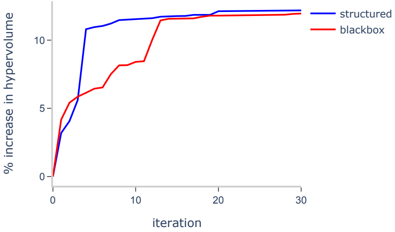
CFR Optimization with ParMOO

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

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

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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Chang and Wild. JOSS 8(82):4468 (2023)

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