ParMOO: A Python library for parallel multiobjective simulation optimization

Scientific Achievement

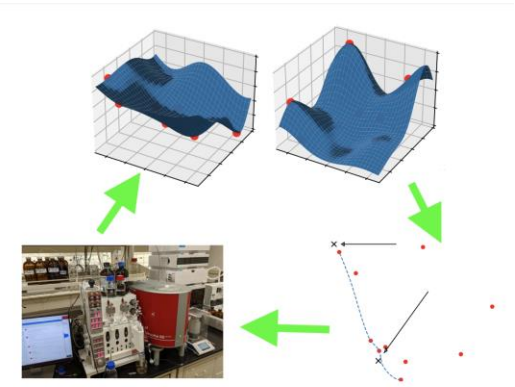
A parallel Python library for customizing and deploying solvers for the optimization of expensive scientific and engineering processes involving multiple conflicting objectives, such as computer simulations and laboratory experiments.

Significance and Impact

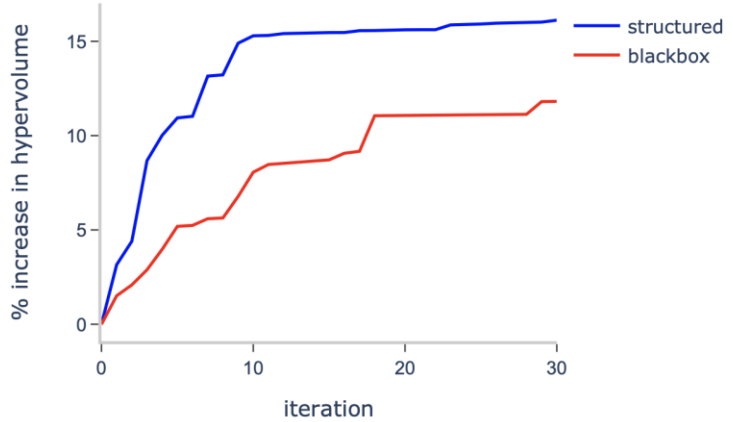
- Easy to deploy in workflows such as HPC systems and self-driving labs
- Combines state-of-the-art techniques from nonlinear optimization, surrogate modeling, data acquisition, design-of-experiments, and representation learning
- Supports complex problem types, including mixed variables and black-box constraints
- Allows scientists to take advantage of domain knowledge and exploit problem structures

Technical Approach

- Combines several existing and novel methodologies for reducing diverse problems to a common form
- Uses modular design and agile methodology for maintainability and extensibility
- Software is open-source and documented with an automated CI/CD pipeline
- Demonstrated the effectiveness of techniques on multiple real-world problems
- Layers over existing ECP software libEnsemble to achieve parallelism on HPCs



A diagram of ParMOO's approach for steering experiments, involving surrogate modeling, multiobjective optimization, and data acquisition in a closed loop.



ParMOO's customized structure-exploiting solvers outperform a typical black-box solver on a material design problem.

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