2024 NETL Workshop on Multiphase Flow Science
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ActivO: A Novel Active Machine Learning Framework for Rapid Simulation-driven Design Optimization

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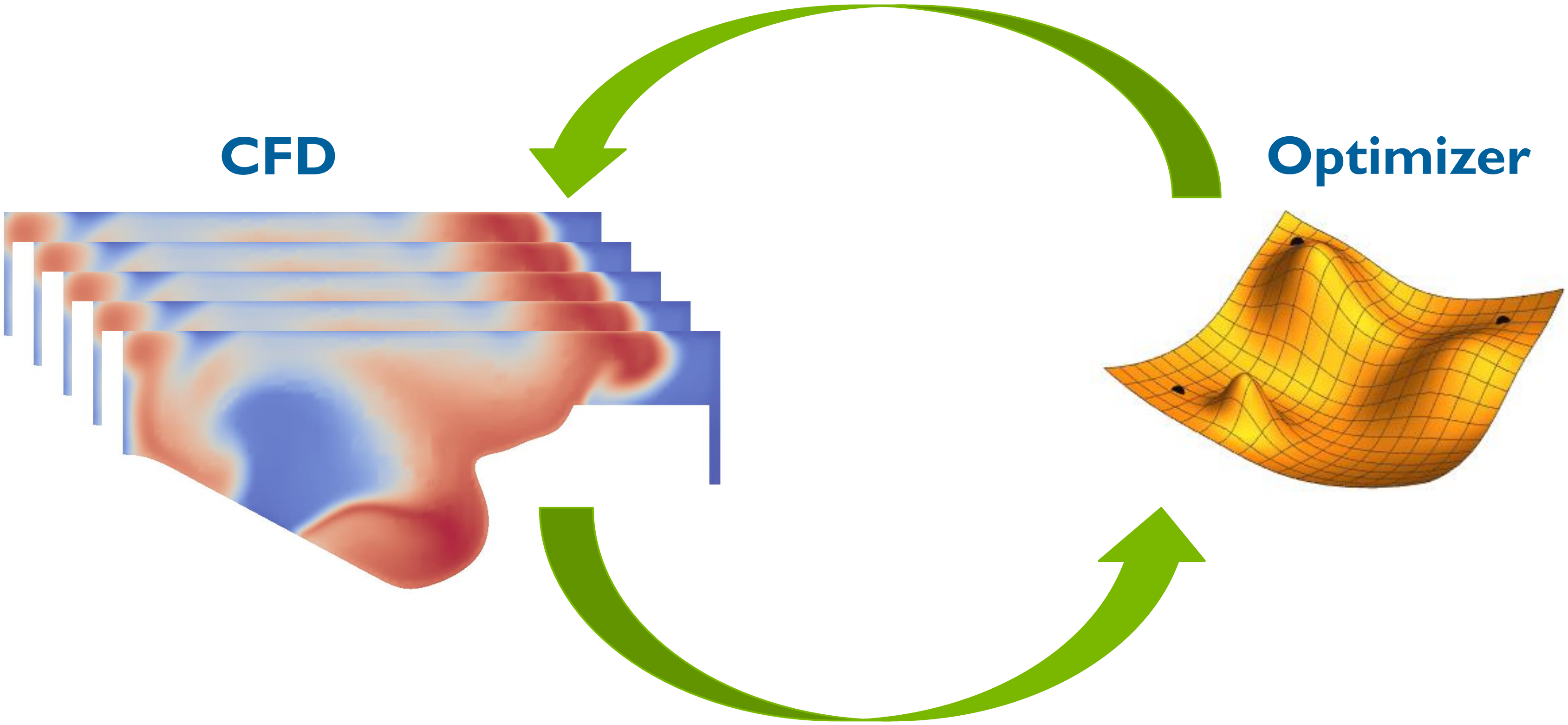
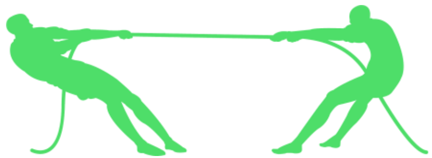
Software Copyright, *SF-19-165*

U.S. patent, ANL-IN-19-103 (*pending*)

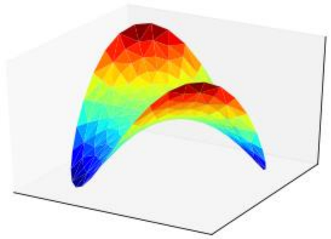
SIMULATION-DRIVEN DESIGN OPTIMIZATION



CHALLENGES OF SIMULATION-DRIVEN DESIGN



Competing objectives



Large multidimensional design spaces (10-20+ control variables)
Highly multi-modal and non-convex response surfaces

CFD simulations can be time-consuming & costly

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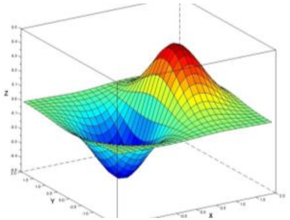
SIMULATION-DRIVEN DESIGN OPTIMIZATION
Conventional approaches

Design of Experiments (DoE)

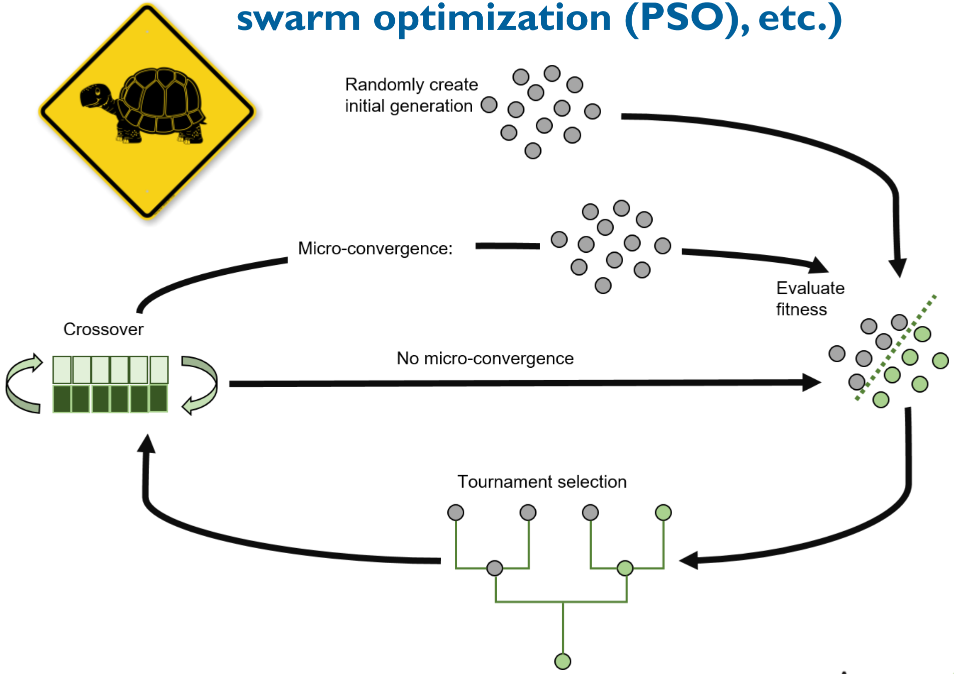
CFD data

↓

Quadratic regression
$y=Ax^2+Bx+C$



Sequential evolutionary algorithms (Genetic algorithm (GA), particle swarm optimization (PSO), etc.)



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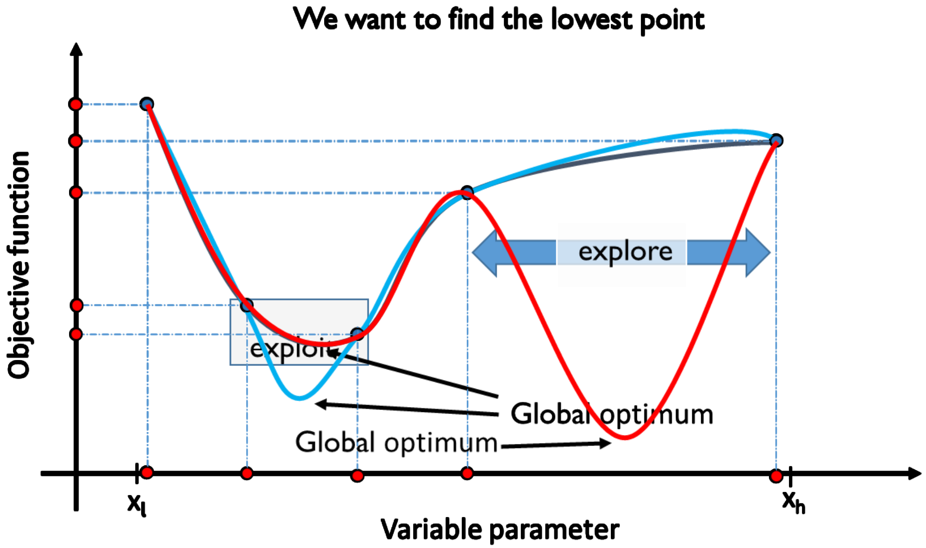
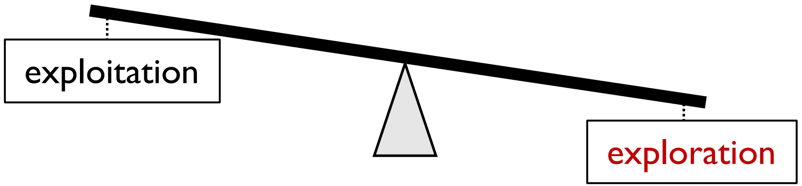
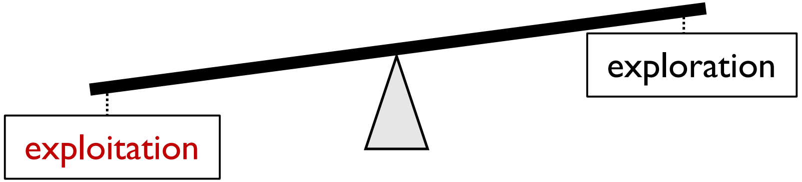
EXPLORATION vs EXPLOITATION OF DESIGN SPACE



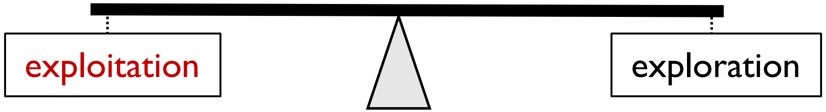
- *Which value of x (design variables) should we run the next batch of simulations?*
- *Goal: Reach global optimum in as few calls to f(x) as possible*



Wasteful; would take longer than needed to reach optimum



The optimizer may converge prematurely

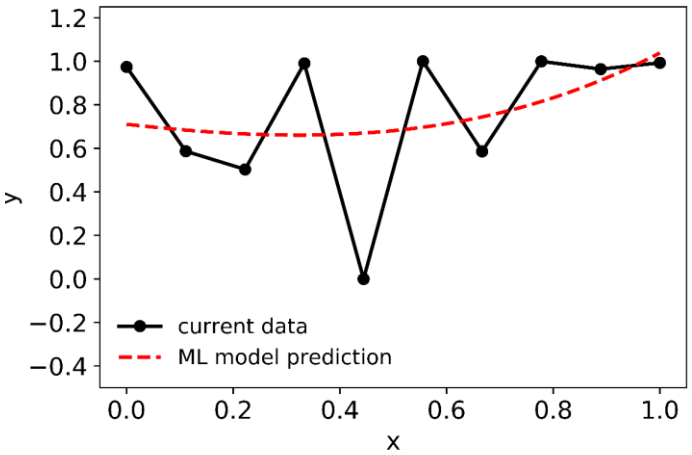


Balanced! Converges to global optimum quickly

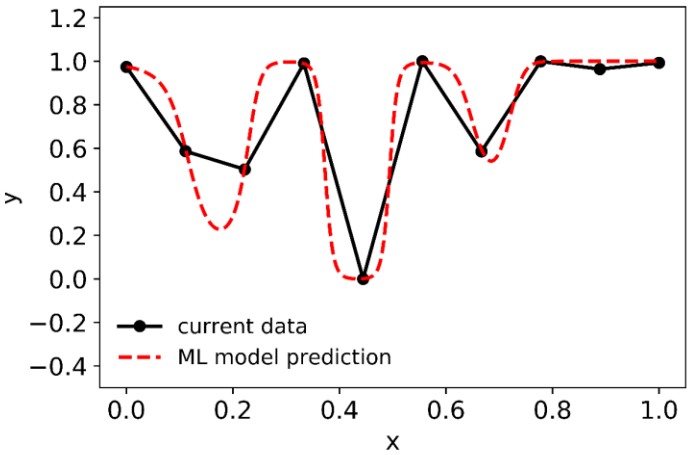
ActivO: COMBINING STRONG AND WEAK LEARNERS

2023 R&D 100 FINALIST

Weak Learner



Strong Learner



- Weak learner gives information about where the promising regions are
- Strong learner provides local surface topology within the promising region

Owoyele & Pal, *ASME J. Energy Resour. Technol.*, 2020

ActivO WORKFLOW

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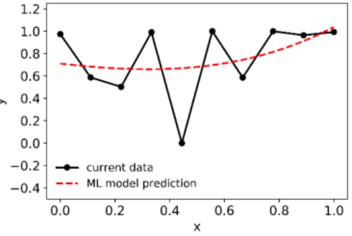
Weak learner
(SVR, BFM, etc.)

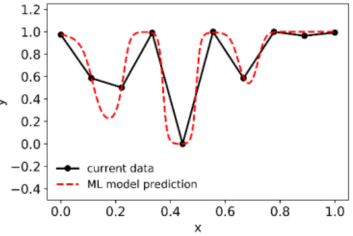
Exploration



Obtain p points with merit values in top kth percentile

Perform N function evaluations (or CFD simulations)

Exploitation



Obtain $(N - p)$ points by running global optimizer

Strong learner
(Committee Machine, RF, XGBoost, etc.)

Feedback new points to function

Owoyele & Pal, *Applied Energy*, 2021

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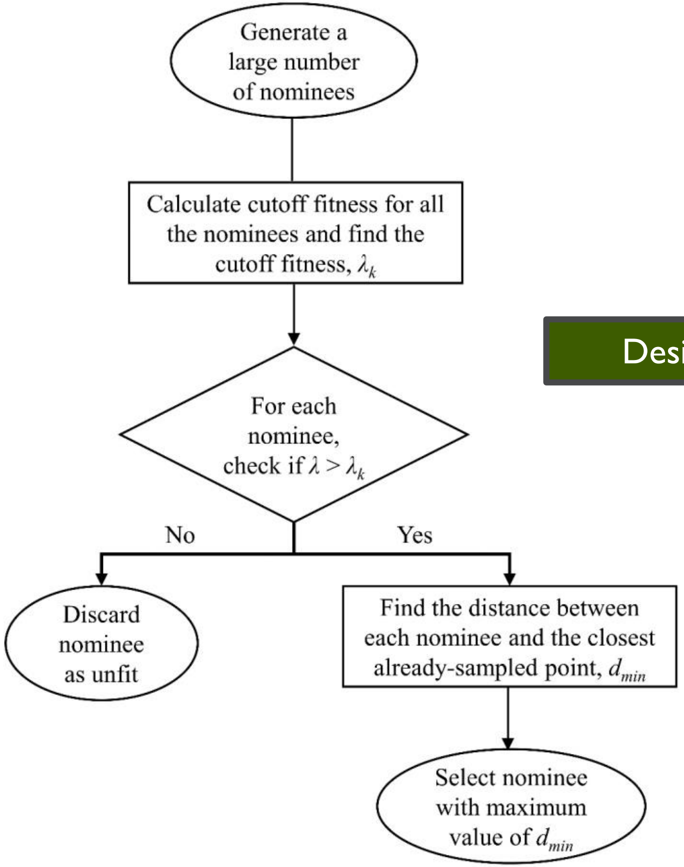
SELECTION OF PROMISING CANDIDATES BY THE WEAK LEARNER



Design space exploration

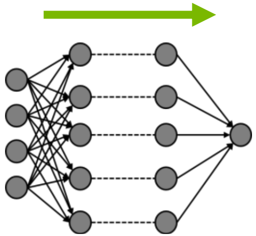
Smart sampling

Owoyele & Pal, *Applied Energy*, 2021

REFINEMENTS (STRONG LEARNER)

Single ANN

input



prediction

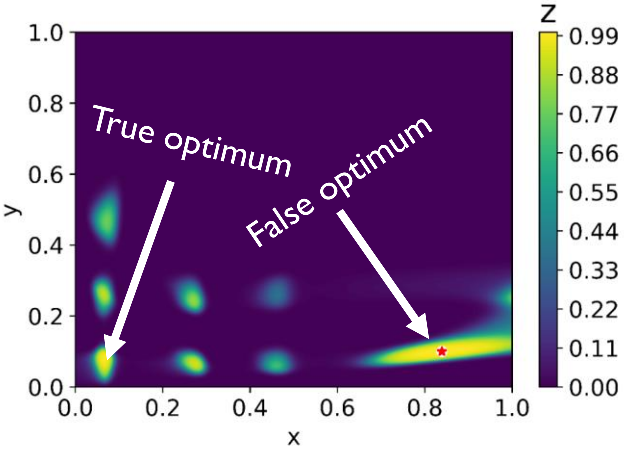
Committee Machine

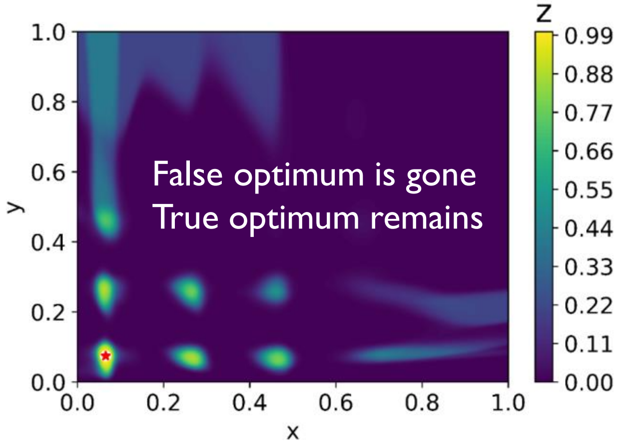
ANN1 | ANN2 | … | ANN *M*

Overall prediction

$$\varphi(x) = \sum_{i=1}^{M} \varphi_i \Big/ M$$

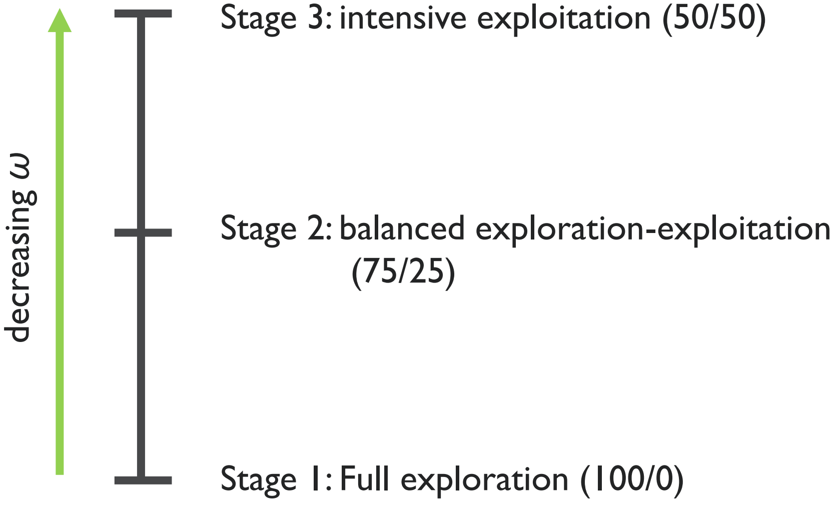
more robust





Owoyele & Pal, *Applied Energy*, 2021

ActivO: DYNAMIC EXPLORATION-EXPLOITATION



The basic idea is to explore "more" in the earlier phases of the optimization process and exploit "more" later as we collect more information

- At the beginning, define several monitor points (M) all over the design surface (M >> N)
- At each iteration, determine the prediction of the weak learner at each of these monitor points, Φ
- Determine the maximum change in the weak learner predictions for monitor points within promising regions:

$$\omega^{i} = \max\left|100 \times \frac{\Phi^{i} - \Phi^{i-1}}{\Phi^{i-1}}\right| \%$$

- This maximum change is defined as ω
- ω gives a measure of how much the weak learner predictions close to the projected global optimum are changing
- If ω increases above 5%, explore more; if it is decreasing, increase exploitation
- Convergence is assumed to occur if ω remains below 5% and the improvement in the best fitness is less than ε for 5 successive iterations

Owoyele & Pal, *Applied Energy*, 2021

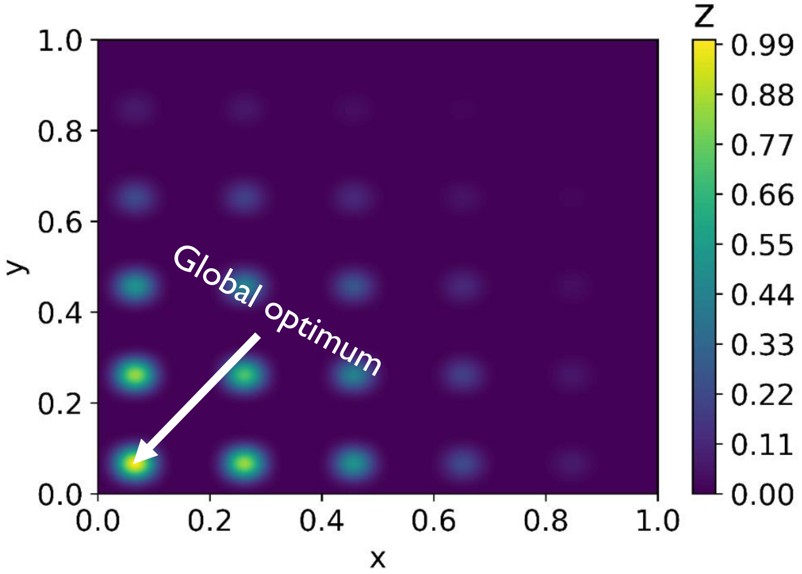
CANONICAL 2D OPTIMIZATION TEST CASE

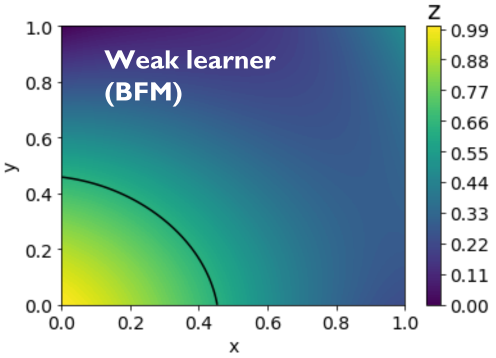
$$f_x = exp\left(\frac{-4\,log\,2\,(x-0.0667)^2}{0.64}\right) sin(5.1\pi x + 0.5)^6$$

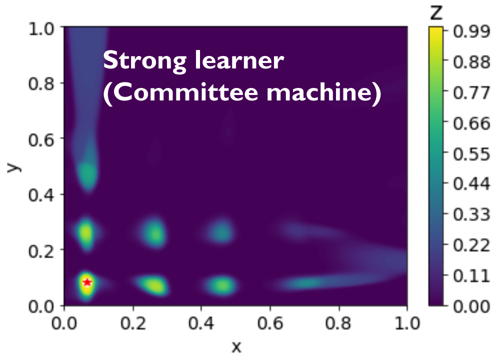
$$f_y = exp\left(\frac{-4\,\log 2\,(y-0.0667)^2}{0.64}\right) \sin(5.1\pi y + 0.5)^6$$

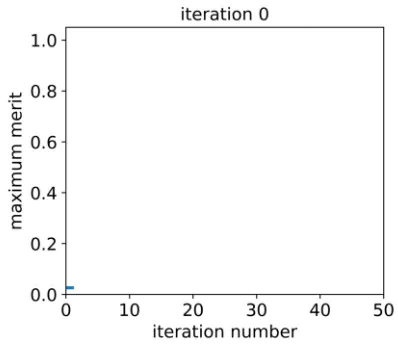
Merit function → $z = f_x f_y$

Maximum z = 1.0 occurring at x = y ≈ 0.0668





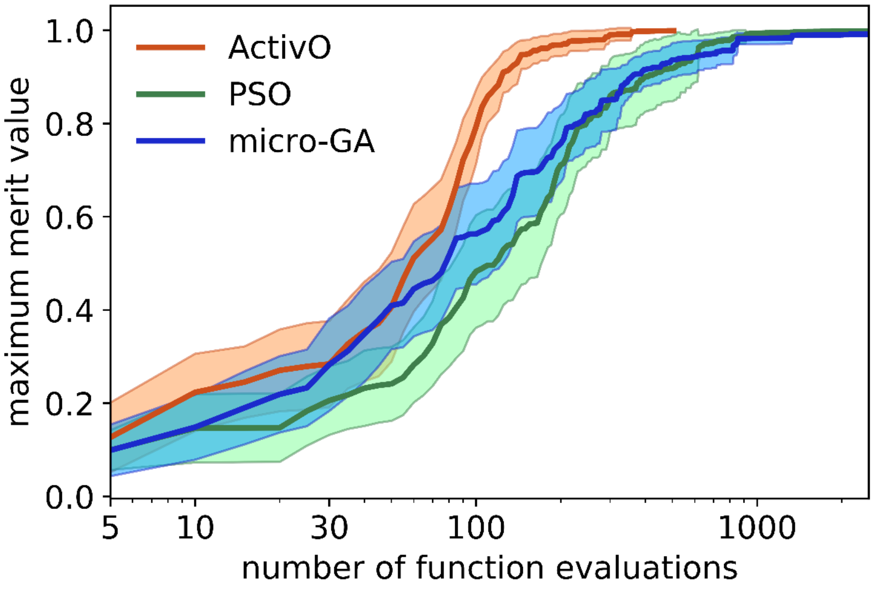


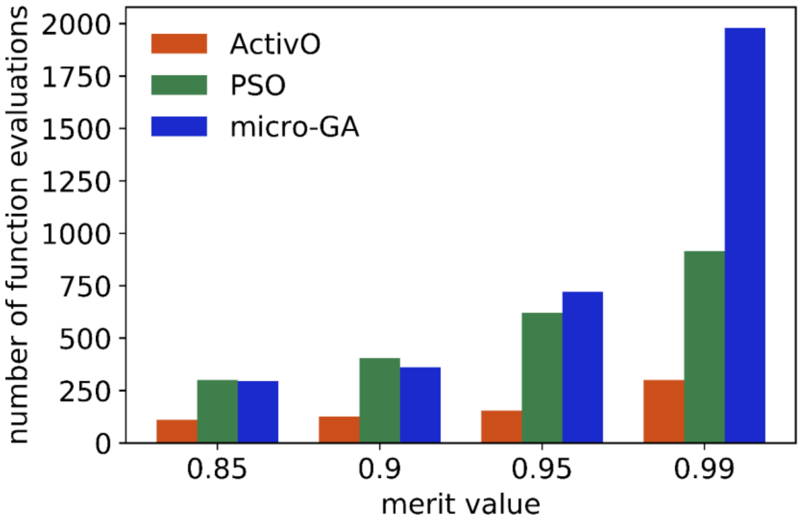


5 function evaluations per iteration

OPTIMIZATION RESULTS

Merit values based on average across 25 trials





- ActivO is ~6 times faster than μGA and ~3 times faster than PSO
- ActivO is more robust than μGA and PSO

Owoyele & Pal, *ASME J. Energy Resour. Technol.*, 2020

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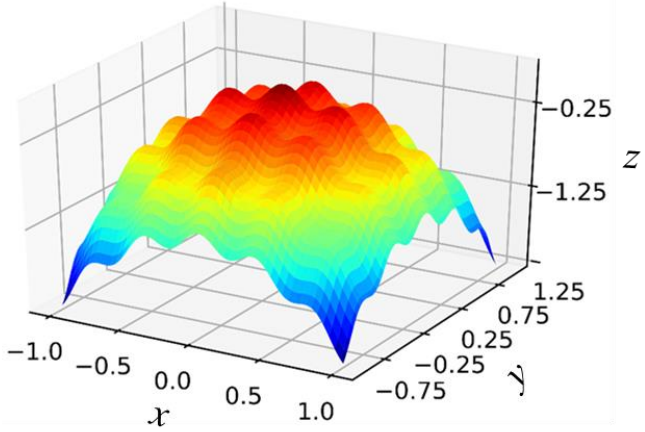
COSINE MIXTURE FUNCTION TEST CASE

$$z = 0.1\,(\cos 5\pi x + \cos 5\pi y) - (x^2 + y^2)$$

$$x \in [-1, 1], y \in [-1, 1]$$

Objective is to maximize z

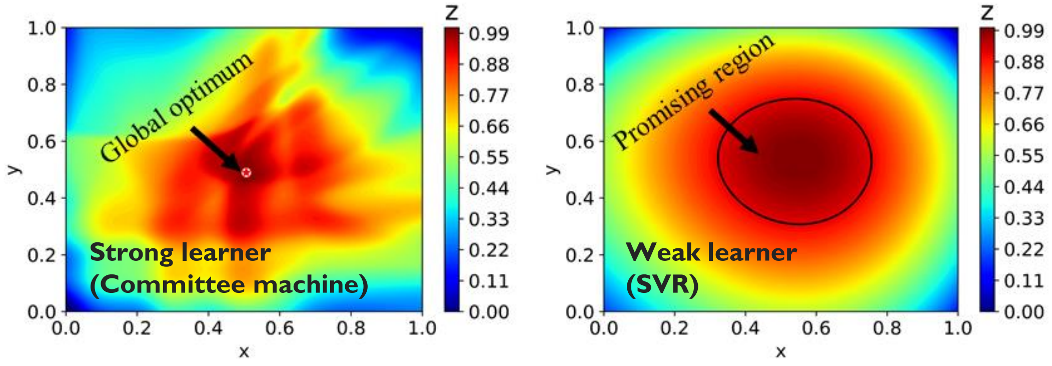
Maximum z (= 0.2) occurs at $x = y = 0$



Owoyele & Pal, *Applied Energy*, 2021

COSINE MIXTURE FUNCTION TEST CASE

After convergence of ActivO



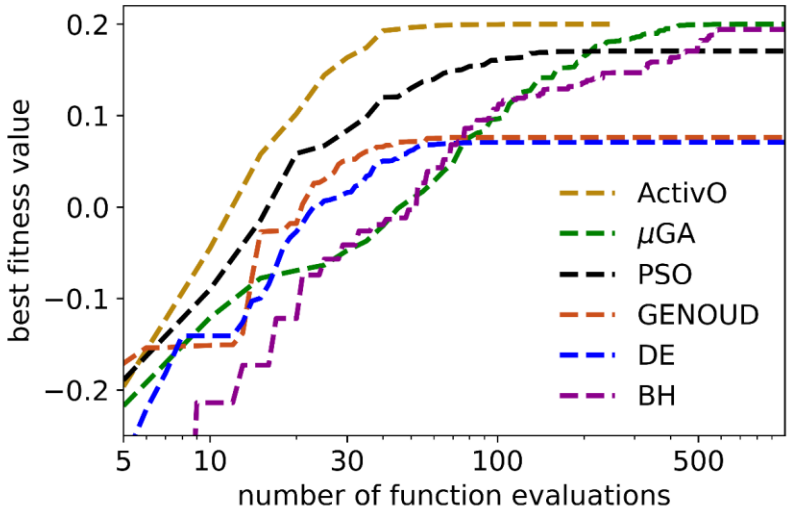
ActivO is compared against 5 state-of-the-art optimizers:

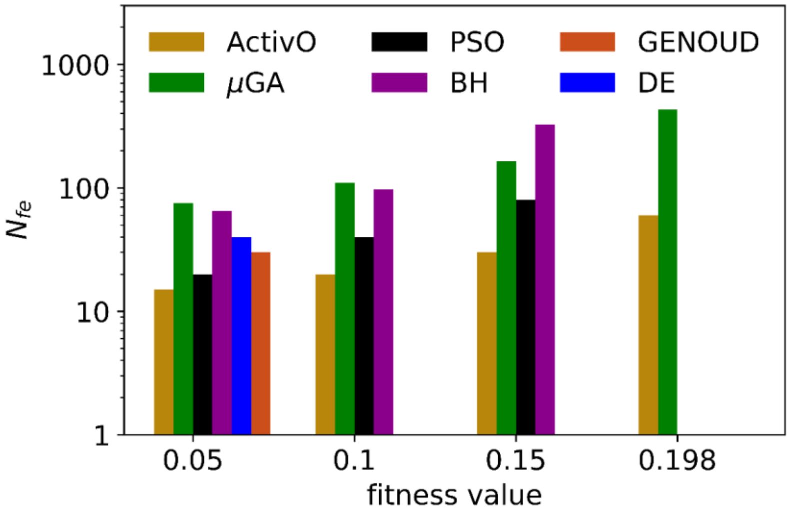
1. Micro-genetic Algorithm (μGA)
2. Particle Swarm Optimizer (PSO)
3. Differential Evolution (DE)
4. Genetic Optimization using Derivatives (GENOUD)
5. Basin Hopping (BH)

Owoyele & Pal, *Applied Energy*, 2021

OPTIMIZATION RESULTS

Merit values based on average across 25 trials





- ActivO converges to the global optimum much faster than all the other optimizers
- PSO, DE, and GENOUD converge prematurely and fail to reach the global optimum

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CFD-DRIVEN IC ENGINE OPTIMIZATION TEST CASE

- Optimization of a heavy-duty engine operating on a gasoline-like fuel at a medium load condition
- Nine-dimensional design space

Notation	Input Parameter	min	max	units
nNoz	**Number of Nozzle holes**	8	10	-
TNA	**Total Nozzle Area**	1	1.3	-
Pinj	**Injection Pressure**	1400	1800	bar
SOI	**Start of injection timing**	-11	-7	dATDC
Nang	**Nozzle Inclusion Angle**	73	83	deg
EGR	**EGR fraction**	0.35	0.5	-
Tivc	**IVC temperature**	323	373	K
Pivc	**IVC pressure**	2.0	2.3	bar
SR	**Swirl Ratio**	-2.4	-1	-

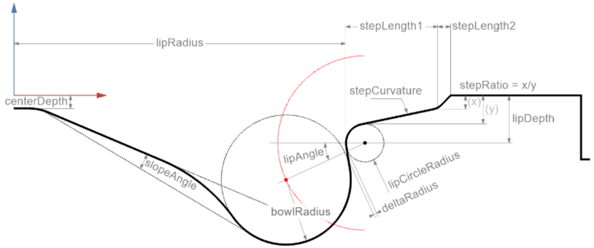
$$Merit = 100 * \left\{ \frac{160}{ISFC} - f(PMAX) - f(MPRR) - f(SOOT) - f(NO_x) \right\}$$

$$f(PMAX) = 100 \begin{Bmatrix} \frac{PMAX}{220} - 1, \text{if PMAX} > 220 \\ 0, \text{if PMAX} \leq 220 \end{Bmatrix}$$

$$f(MPRR) = 10 \begin{Bmatrix} \frac{MPRR}{15} - 1, \text{if MPRR} > 15 \\ 0, \text{if MPRR} \leq 15 \end{Bmatrix}$$

$$f(SOOT) = \begin{Bmatrix} \frac{SOOT}{0.0268} - 1, \text{if SOOT} > 0.0268 \\ 0, \text{if SOOT} \leq 0.0268 \end{Bmatrix}$$

$$f(NO_x) = \begin{Bmatrix} \frac{NO_x}{1.34} - 1, \text{if } NO_x > 1.34 \\ 0, \text{if } NO_x \leq 1.34 \end{Bmatrix}$$



Shape optimization and multiple loads can also be incorporated (ASME JERT-20-1594, SAE 2020-01-1313)

Owoyele & Pal, *Applied Energy*, 2021

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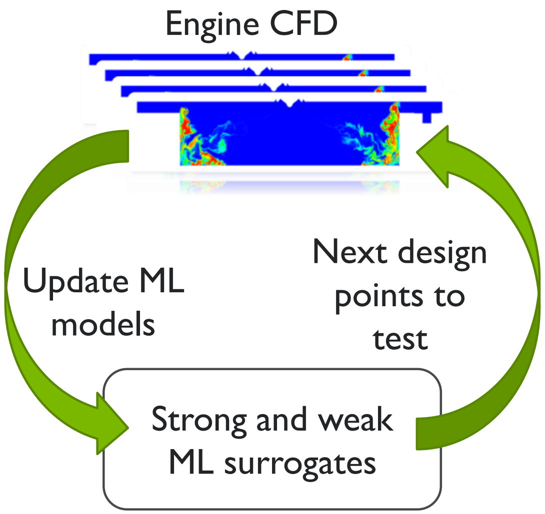
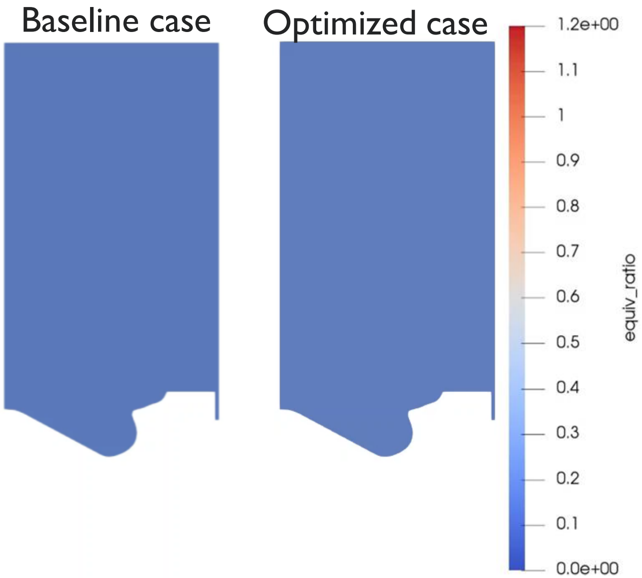
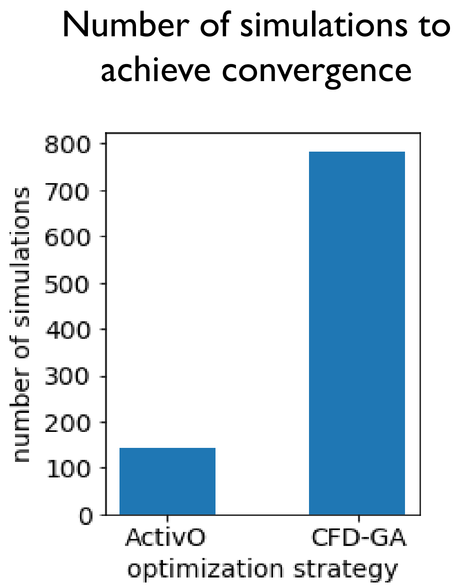
OPTIMIZATION RESULTS



***ActivO was coupled with CONVERGE CFD solver**

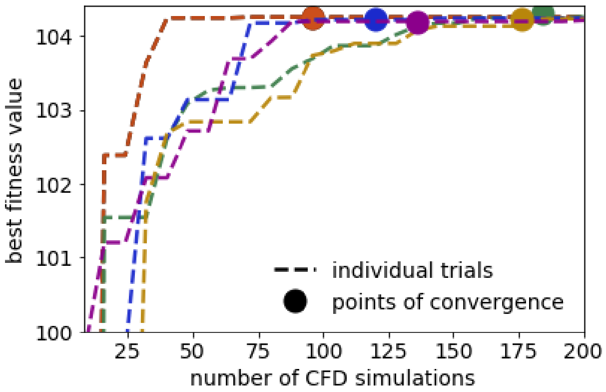


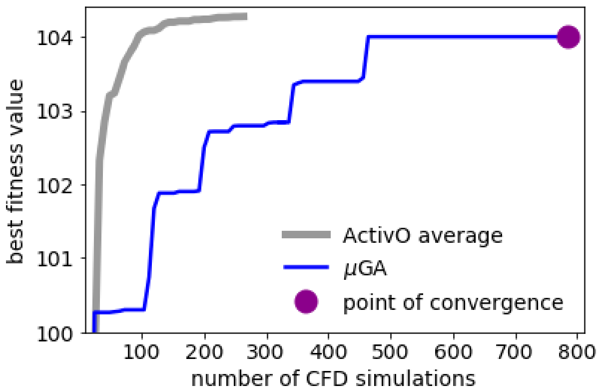


- ActivO lowers computational expense from 117,000 core hours to 20,000 core hours (over 80% decrease)
- ActivO shows 5-7X speedup (from 2 months to less than 2 weeks) over CONVERGE's μGA algorithm

OPTIMIZATION RESULTS

- 8 CFD simulations/design iteration





➢ Number of CFD simulations it takes to reach a merit value of 104.0:
   - 88 for ActivO vs 464 for μGA

➢ Maximum merit value reached:
   - 104.14 for ActivO vs 104.0 for μGA

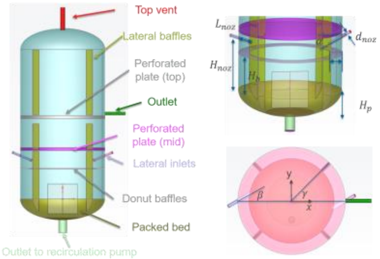
Owoyele & Pal, *Applied Energy*, 2021

CFD-ActivO DESIGN OPTIMIZATION

Multi-parameter optimization of turbulent mixer geometry

1

Turbulent jet mixer geometry



10-parameter design space

$$MF = \frac{entrained\ \%_{ref}}{entrained\ \%} + \frac{mixing\ time}{mixing\ time_{ref}} + f(\tau_{bub})$$

- Evaluate the performance of mixer designs (multi-parameter)
- Generate new promising sets of design parameters

ActivO

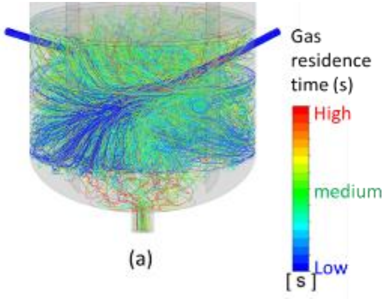
Active ML optimization tool

3

2

OpenFOAM®

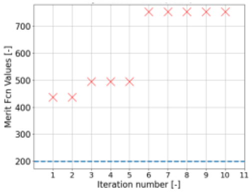
- Automatic mesh generation and CFD case setup
- Multiphase L-E CFD simulations

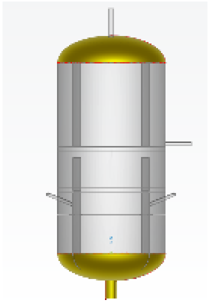


4

CAESES

Automatic geometry morphing for the new design parameter sets obtained from ActivO





Asztalos et al., APS-DFD, 2023

Asztalos et al., APS-DFD, 2024

Argonne collaborators: Lorenzo Nocivelli, Katherine Asztalos
Dow Collaborators: Chi-Wei Tsang, Mehdi Khalloufi

SUMMARY

- An adaptive surrogate-based active ML optimization algorithm (ActivO) was developed that uses a weak learner for exploration and a strong learner for exploitation of the design space
- A mechanism for dynamically adjusting the balance between exploration and exploitation, as well as a method for assessing convergence was incorporated
- ActivO was also shown to converge significantly faster to the design optimum compared to state-of-the-art optimization algorithms; this leads to significant savings in the design time and associated computational cost
- Demonstration studies have been performed for optimization of IC engines and turbulent jet mixers wherein ActivO was coupled with CONVERGE and OpenFOAM CFD solvers, respectively
- The self-contained and automated ActivO software can be readily interfaced with any CFD code of interest for performing a wide range of design optimization campaigns

Future work

- Incorporation of uncertainty-based robust optimization strategies to account for perturbations and/or manufacturing tolerances in the design parameters
- Parallelized workflows for large-scale optimization campaigns via coupling with SmartSim

PUBLICATIONS & PRESENTATIONS

- O. Owoyele and P. Pal, "A novel machine learning-based optimization algorithm (ActivO) for accelerating simulation-driven engine design", *Applied Energy*, Vol. 285, pp. 116455, 2021.

- O. Owoyele and P. Pal, "A novel active optimization approach for rapid and efficient design space exploration using ensemble machine learning", *Journal of Energy Resources Technology*, Vol. 143(3), pp. 032307, 2020.

- K.J. Asztalos, L. Nocivelli, P. Pal, C-W. Tasang, and M. Khalloufi, "An end-to-end framework coupling CFD and active machine learning optimizer (ActivO) for rapid simulation-driven design of turbulent jet mixers", *76th Annual Meeting of the APS Division of Fluid Dynamics*, 2023.

- K.J. Asztalos, L. Nocivelli, P. Pal, C-W. Tasang, and M. Khalloufi, "Design optimization of turbulent jet mixers utilizing active machine learning optimization (ActivO)", *77th Annual Meeting of the APS Division of Fluid Dynamics*, 2024 (submitted).

THANK YOU

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