Outlier-aware Multi-fidelity Surrogate-based Hyperparameter Optimization for Topology Optimization

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※ TO: topology optimization
※ SIMP: solid isotropic material with penalization

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1-1. Topology optimization and local optima

❖ Density-based topology optimization (TO)

- SIMP relaxes the binary (0/1) material layout into continuous densities for gradient-based search.[1]
- The relaxed problem remains non-convex, so the optimizer is easily trapped in local optima.

❖ Sensitivity to hyperparameters

- A small change in the penalty parameter p leads to a markedly different optimal topology.



(a) (b) (c) (d)

Cantilever beam: (a) problem setup and optimal topologies for (b) p = 3, (c) p = 4, (d) p = 5

Hyperparameter settings determine which local optimum is reached

[1] O. Sigmund, J. Petersson, Numerical instabilities in topology optimization: a survey on procedures dealing with checkerboards, mesh-dependencies and local minima, *Struct. Optim.* 16 (1998) 68-75.

※ TO: topology optimization
※ LF: low-fidelity
※ HF: high-fidelity

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1-2. Limitations of existing approaches

❖ Approaches to mitigate the local optimum issue in TO

- Existing approaches either increase computational cost or rely on many repeated full TO runs.

Category	Representative strategy	Limitation
Global search	Genetic algorithm, simulated annealing	**High computational cost** for large-scale problems
Revised local search	Continuation, deflation	**Discontinuous paths**, parameter sensitivity
Data-driven: density level	Density field → objective (deep neural networks)	**Many completed TO runs** needed for training
Data-driven: hyperparameter level	Surrogate over TO hyperparameters[2]	**Gray, infeasible designs** contaminate learning
Data-driven: LF → HF	Optimize with LF model, re-evaluate with HF model	Search stays in LF space, **no unified MF formulation**

A data-driven framework tailored to TO is required: lower cost, same accuracy

[2] Ha, D., & Carstensen, J. (2024). Automatic hyperparameter tuning of topology optimization algorithms using surrogate optimization. *Struct. Multidiscip. Optim.*, 67, 157.

※ SF: single-fidelity
※ MF: multi-fidelity
※ HF: high-fidelity
※ LF: low-fidelity

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1-3. Surrogate modeling and multi-fidelity approach

❖ Surrogate model

- A surrogate model is a cheap approximation of an expensive simulation built from a limited number of samples.
- It replaces repeated simulations during optimization.

❖ Multi-fidelity (MF) surrogate model

- It combines abundant, cheap LF data with sparse, accurate HF data.
- LF data capture the global trend, and HF data calibrate it.

❖ Sequential sampling

- An acquisition function selects the next HF sample to refine the model.

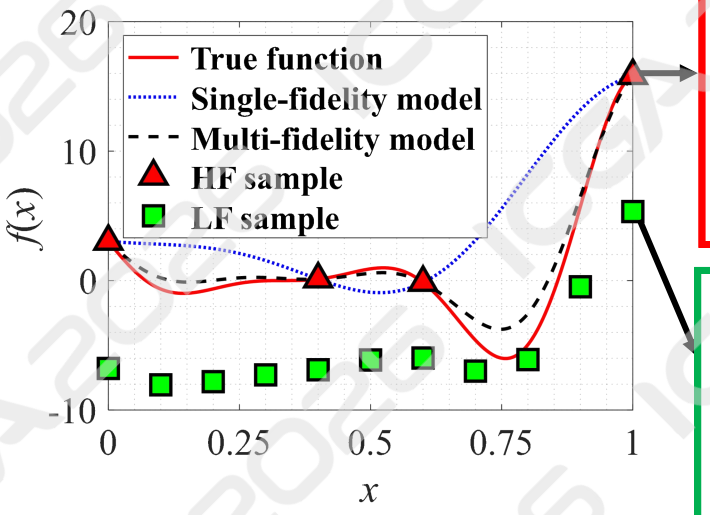
Samples $\mathbf{x}_1, \ldots, \mathbf{x}_n$ → **Simulation** $f(\mathbf{x}_i)$: expensive → **Surrogate** $\hat{y}(\mathbf{x}) \approx f(\mathbf{x})$: fast

Basic formulation of MF model

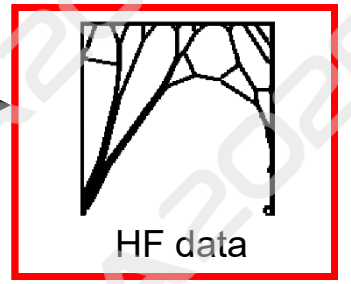
Correction term

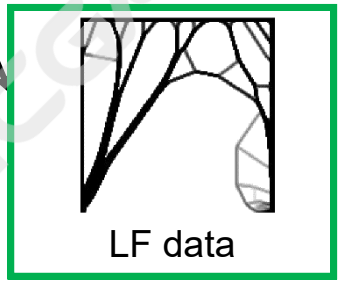
$$\hat{y}_{\mathrm{MF}}(\mathbf{x}) = \rho \hat{y}_{\mathrm{LF}}(\mathbf{x}) + \hat{\delta}(x)$$

Trend term



MF modeling





Benefits of MF surrogate model:
Higher accuracy than SF models under the same HF budget

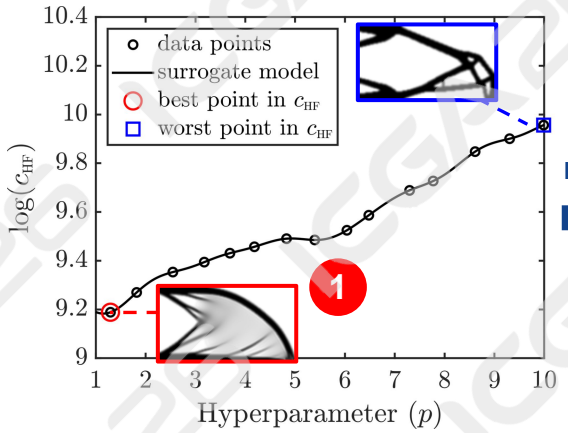
※ HF: high-fidelity
※ LF: low-fidelity

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1-4. Research motivation

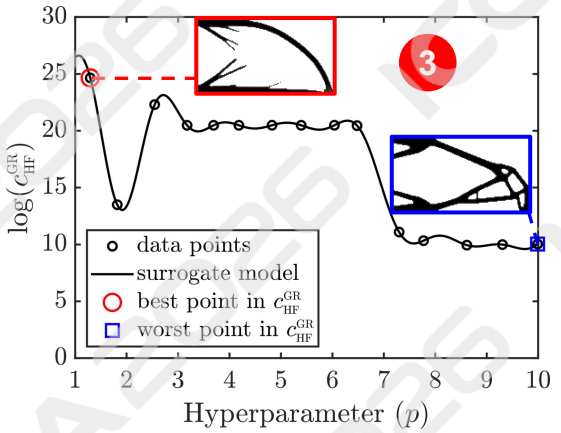
Original response | **Refined response**

HF data



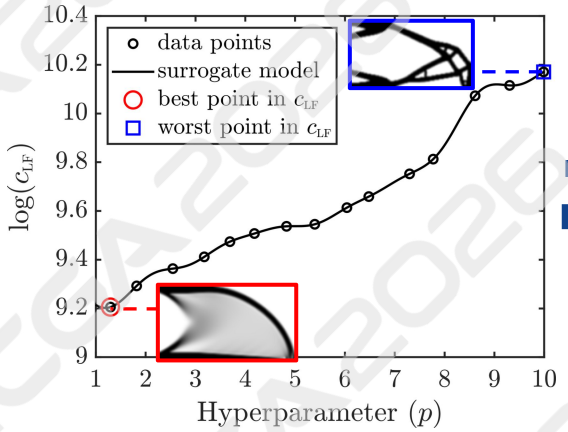
Gray removal

2

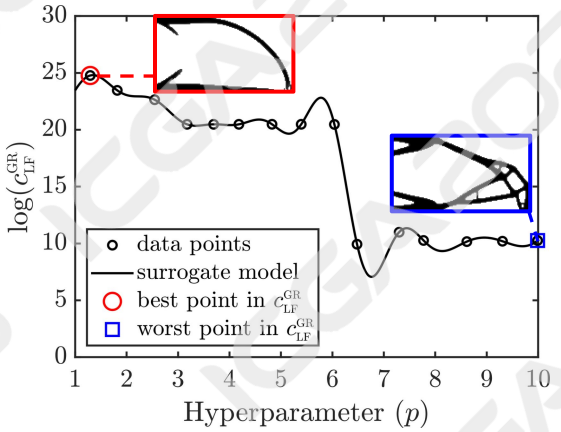


4 ▲▼ LF and HF show similar trends

LF data



Gray removal



Key observations

1. The original best design (red) is dominated by gray regions.
2. After gray removal, the red design becomes one of the worst.
3. Refined responses span a wide range, so HF samples in high-compliance regions are wasted.
4. Refined LF responses reproduce the refined HF trend at a much lower cost.

Refined LF data detect outlier regions early and keep HF samples away from them

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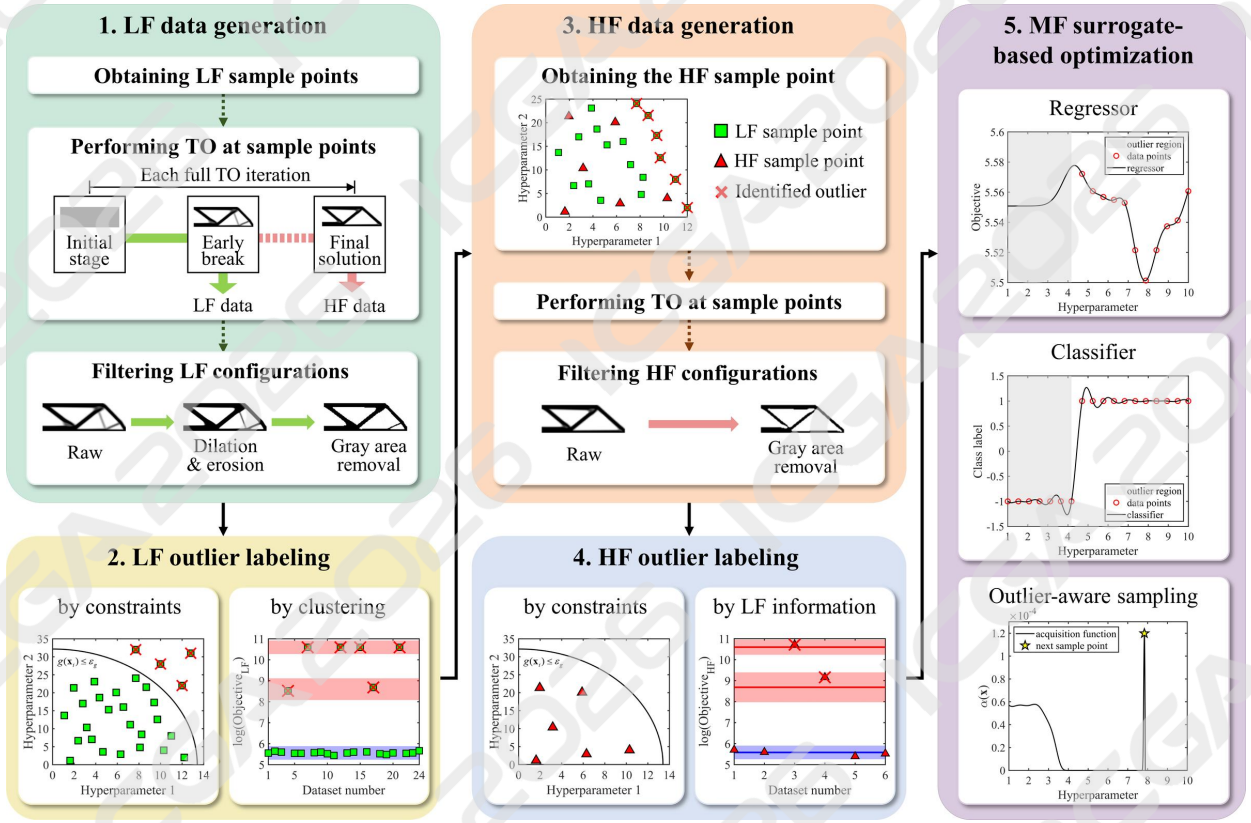
※ TO: topology optimization
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2-1. Overview of the proposed framework

❖ Outlier-aware MFTO in the hyperparameter design space:

- Outliers are detected, labeled and exploited from data generation to optimization.[*]



1. LF data generation
Early-terminated TO + filtering

2. LF outlier labeling
Constraints + clustering

3. HF data generation
LF-guided design of experiments

4. HF outlier labeling
Guided by LF cluster centroids

5. MF surrogate-based optimization
Inlier regressor + outlier classifier

Conceptual illustration of the proposed MFTO framework

[*] Park, J., Lee, M., & Lee, I. (2026). Outlier-aware multi-fidelity surrogate-based hyperparameter optimization for topology optimization. *Computers & Structures*, 333, 108476.

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2-2. Low-fidelity data generation

❖ Early termination of TO

- Convergence tolerance: 10^{-3} is used for LF, whereas 10^{-6} is used for HF (L_2 norm of design change).
- Later iterations mainly refine boundaries, so early results still reveal the global trend.

❖ Filtering for refined responses

- LF only: dilation (η = 0.35) and erosion (η = 0.65) reinforce the structural backbone.
- LF and HF: gray-area removal sets $0.05 < \tilde{x} < 0.95$ to 0 before compliance is evaluated.

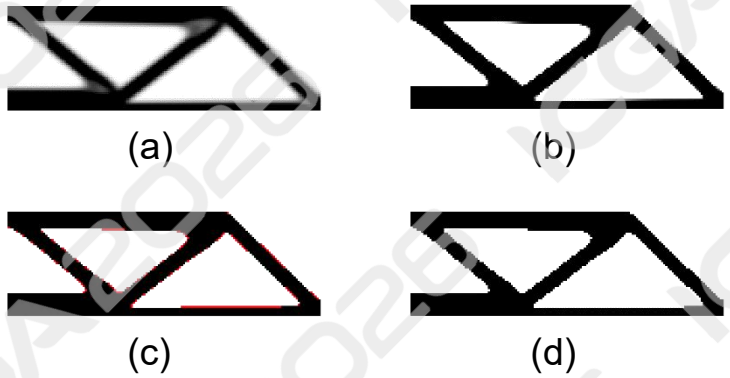
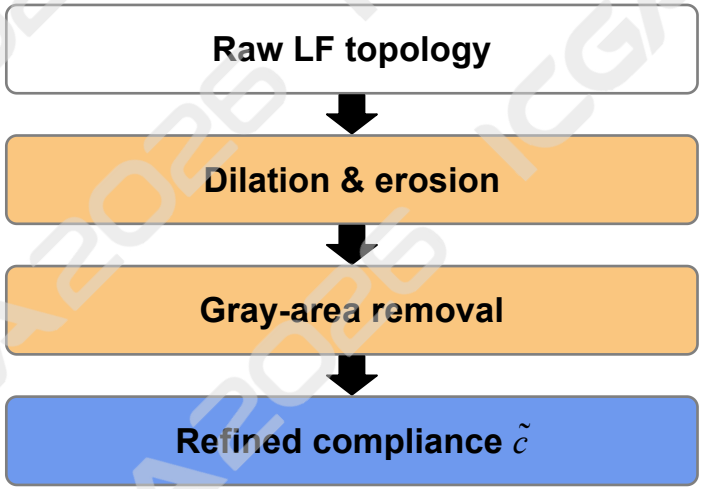


Illustration of the density filtering process:
(a) Original, (b) filtered, (c) gray regions, (d) refined



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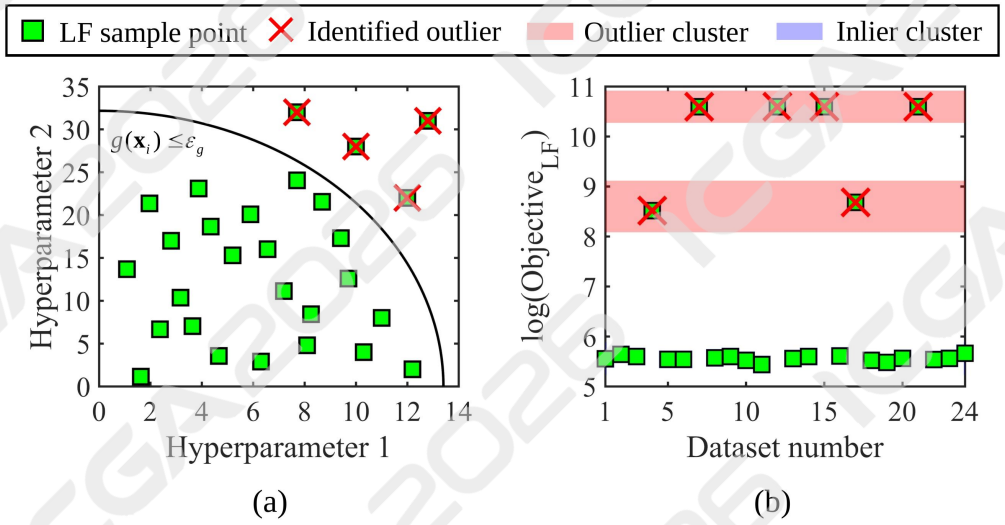
2-3. Low-fidelity outlier labeling

❖ Two types of outliers

- **Type 1 (constraint violation):** the normalized constraint $g(\mathbf{x}_i) = G(\mathbf{x}_i) / \bar{G} - 1$ exceeds $\varepsilon_g = 0.05$.
- **Type 2 (structural instability):** compliance becomes abnormally large after gray removal.

❖ Recursive binary k-means clustering

- A split is accepted only if the mean silhouette score exceeds 0.7.
- The cluster with the smallest centroid is labeled as the LF inlier set.



(a) Constraint-based and (b) clustering-based detection

LF outlier labeling procedure

Remove samples with $g(\mathbf{x}_i) > \varepsilon_g$

↓

Split the rest by binary k-means

↓

Accept the split if silhouette > 0.7

↓

Lowest-centroid cluster → LF inliers

Steps 2–3 are repeated recursively.

※ HF: high-fidelity
※ LF: low-fidelity

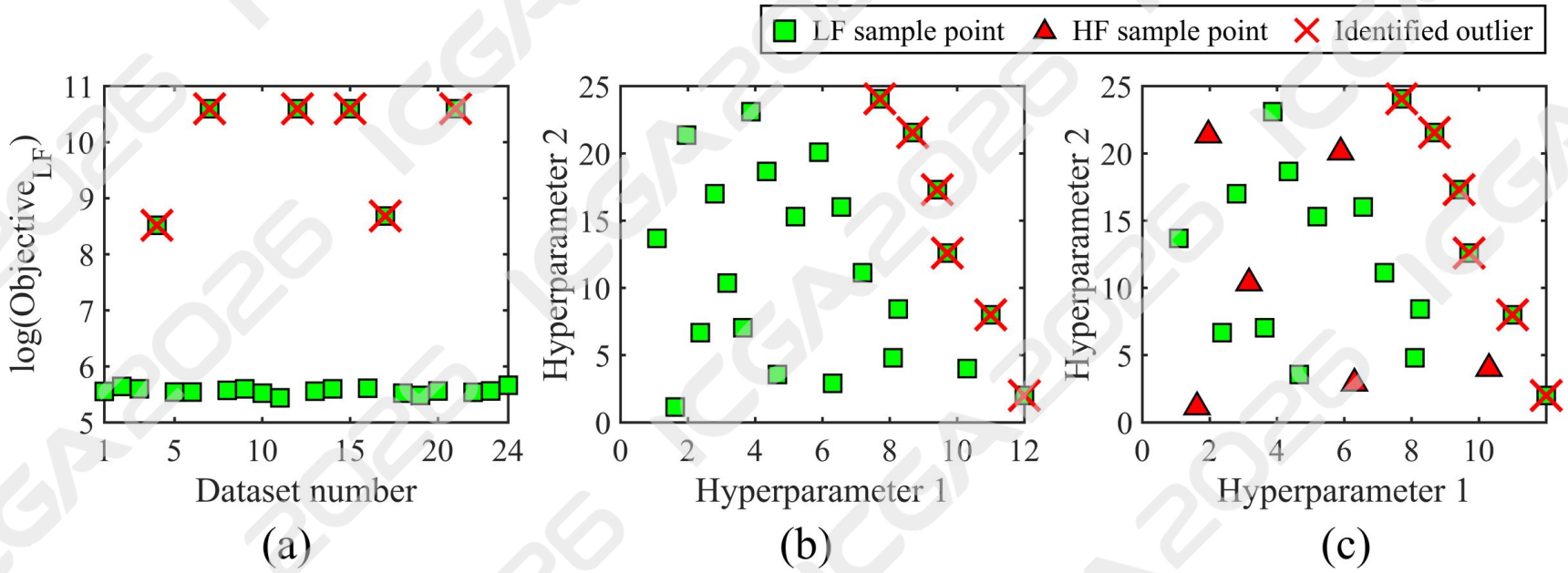
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2-4. LF-guided HF design of experiments

❖ Space-filling HF sampling within the LF inlier region

- LF outliers cluster in specific regions of the input space, which are unpromising for HF.
- HF points are chosen only from LF inlier inputs by maximizing the minimum distance.

$$\mathbf{X}_{\mathrm{HF}} = \arg\max \ \min_{p \neq q} d(\mathbf{x}_{\mathrm{HF}}^{(p)}, \mathbf{x}_{\mathrm{HF}}^{(q)}), \quad \mathbf{X}_{\mathrm{HF}} \subset \mathbf{X}_{\mathrm{LF,in}}$$



(a) LF outliers, (b) outliers in the input space, (c) HF points selected from promising LF samples

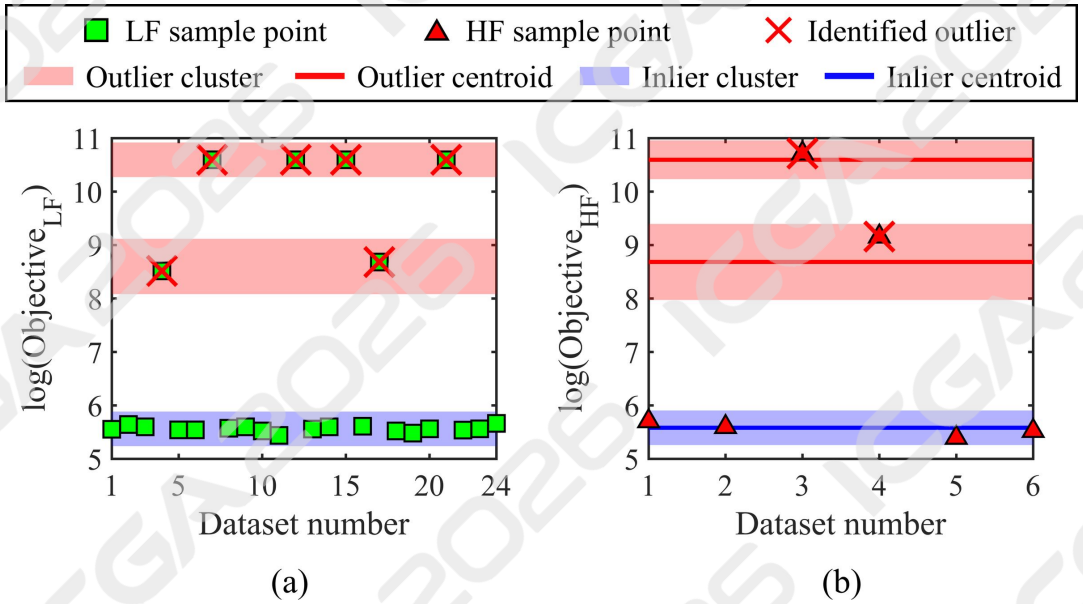
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2-5. LF-guided HF outlier labeling

❖ Labeling limited HF data with LF information

- Too few HF samples are available for direct clustering.
- Constraint-violating HF samples are removed with the same criterion as LF.
- Each HF sample is assigned to the nearest LF cluster centroid in objective value.



(a) LF clustering and (b) HF labeling via LF centroids

$$C(\mathbf{x}_i^{\mathrm{HF}}) = \arg\min_k |y_i^{\mathrm{HF}} - \bar{\mu}_k^{\mathrm{LF}}|$$

$$D_{\mathrm{in}}^{\mathrm{HF}} = \{\mathbf{x}_i^{\mathrm{HF}} \mid C(\mathbf{x}_i^{\mathrm{HF}}) = k_{\mathrm{in}}^{*}\}$$

$\bar{\mu}_k^{\mathrm{LF}}$: **centroid of the k-th LF cluster**

k_{in}^{*}: **LF cluster with the smallest centroid**

$D_{\mathrm{in}}^{\mathrm{HF}}$: **HF inlier set**

HF outliers are labeled without clustering the scarce HF data

[*] Park, J., Lee, M., & Lee, I. (2026). Outlier-aware multi-fidelity surrogate-based hyperparameter optimization for topology optimization. *Computers & Structures*, 333, 108476.

※ MF: multi-fidelity
※ EI: expected improvement
※ GP: Gaussian process

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2-6. Outlier-aware MF surrogate-based optimization

❖ Two surrogates with different roles

- **Regressor:** a hierarchical MF model is trained only on LF and HF inliers.
- **Classifier:** a GP classifier is trained on all LF and HF labels (inlier 1, outlier −1).

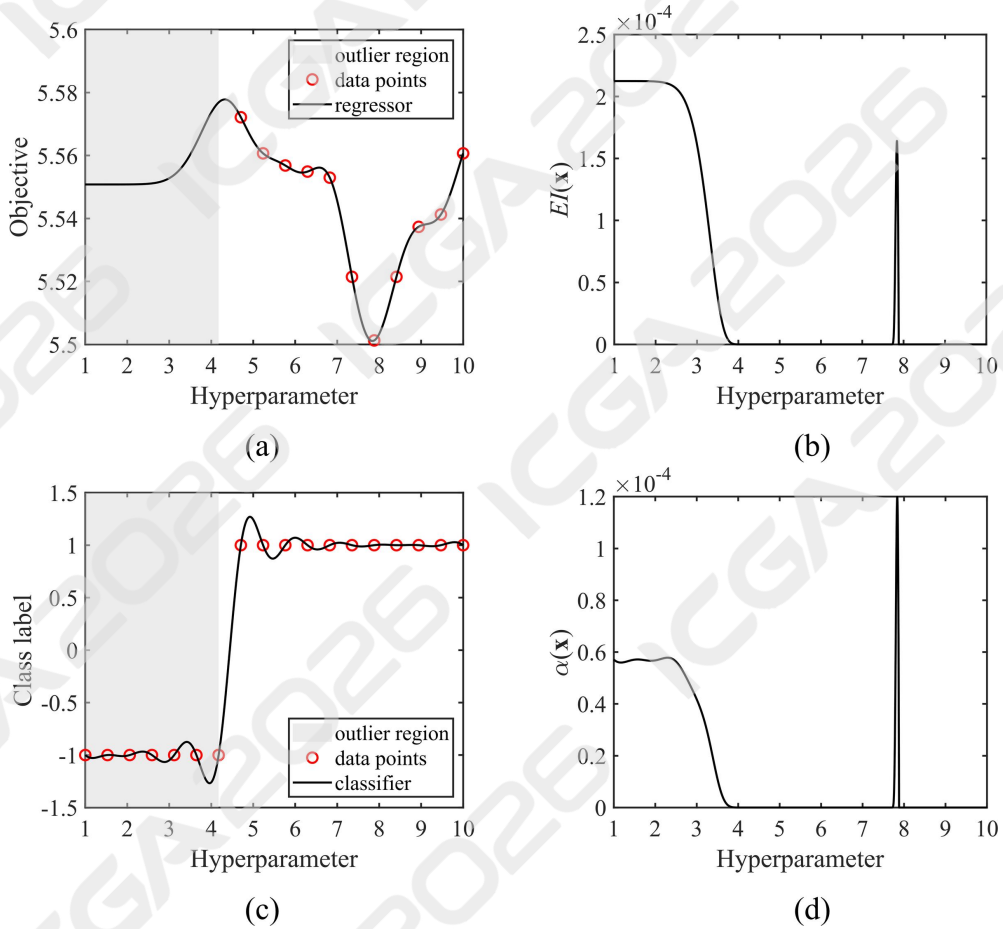
❖ Outlier-aware acquisition function

- EI alone favors empty outlier regions, so it is multiplied by the inlier probability.

$$\alpha(\mathbf{x}) = p_{\text{in}}(\mathbf{x})\, EI(\mathbf{x})$$
$$p_{\text{in}}(\mathbf{x}) = 1 / [1 + \exp(-f_{\text{cls}}(\mathbf{x}))]$$

$f_{\text{cls}}(\mathbf{x})$: GP classifier output, p_{in}: inlier probability

Sampling avoids outlier regions



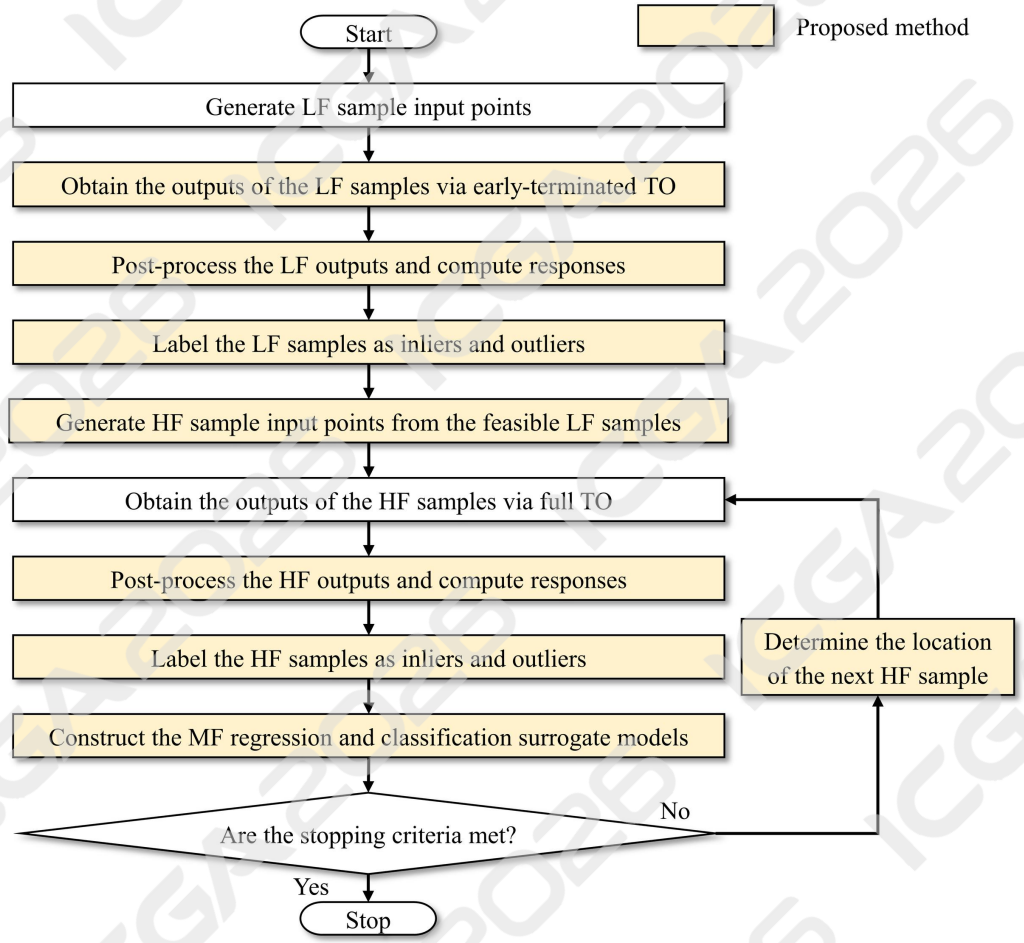
(a) MF regressor, (b) EI, (c) classifier, (d) proposed $\alpha(\mathbf{x})$

[*] Park, J., Lee, M., & Lee, I. (2026). Outlier-aware multi-fidelity surrogate-based hyperparameter optimization for topology optimization. *Computers & Structures*, 333, 108476.

※ HF: high-fidelity
※ LF: low-fidelity

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2-7. Overall procedure



Flowchart of the proposed MFTO framework

❖ Initial stage (Steps 1–8)

- LF: samples from LHS undergo early-terminated TO, refinement and labeling.
- HF: samples from LF-guided DoE undergo full TO, refinement and labeling.

❖ Sequential stage (Steps 9–11)

- The MF regressor and classifier are constructed.
- HF samples are added by maximizing $\alpha(\mathbf{x})$ until the stopping criteria are met.

❖ Computational cost

- TO runs dominate the cost, while surrogate modeling and GA search take only seconds.

[*] Park, J., Lee, M., & Lee, I. (2026). Outlier-aware multi-fidelity surrogate-based hyperparameter optimization for topology optimization. *Computers & Structures*, 333, 108476.

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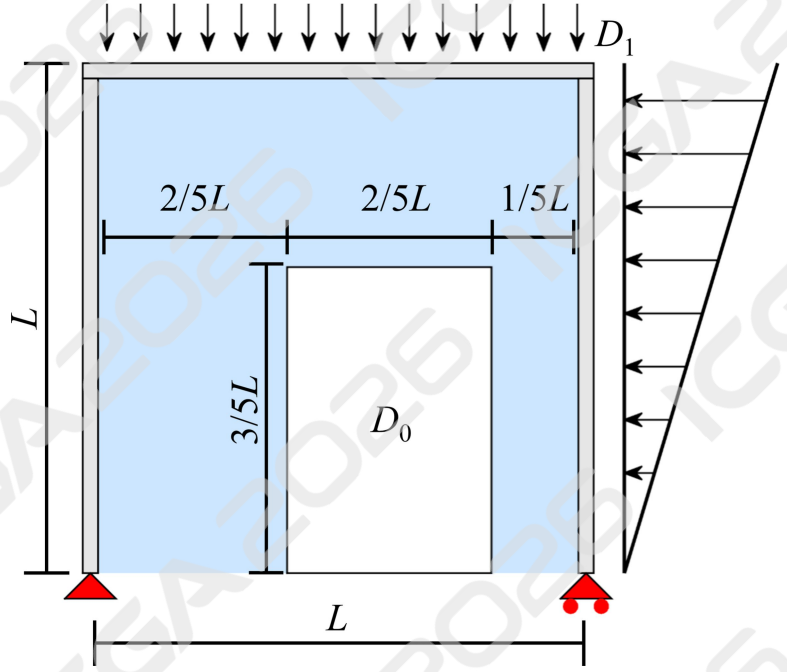
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3-1. Frame reinforcement problem

❖ Numerical example 1: compliance minimization

- The domain has 150 × 150 elements, a volume fraction of 0.2, a fixed boundary D_1 and a void region D_0.
- Six SIMP hyperparameters are optimized, with continuation applied to p and β.



Frame reinforcement problem

Hyperparameter	Bounds	Reference[1]
Initial penalty, p_{ini}	1 – 10	3
Final penalty, p_{final}	3 – 10	3
Initial filter, β_{ini}	1 – 50	2
Final filter, β_{final}	1 – 50	2
Move limit, $move$	0.05 – 0.15	0.1
Initial guess, x_0	0.1 – 0.9	0.2

Hyperparameters and their bounds

[1] Andreassen, E., Clausen, A., Schevenels, M., Lazarov, B. S., & Sigmund, O. (2011). Efficient topology optimization in MATLAB using 88 lines of code. Struct. Multidiscip. Optim., 43, 1-16.

※ SF: single-fidelity
※ MF: multi-fidelity
※ DoE: design of experiments
※ BO: Bayesian optimization

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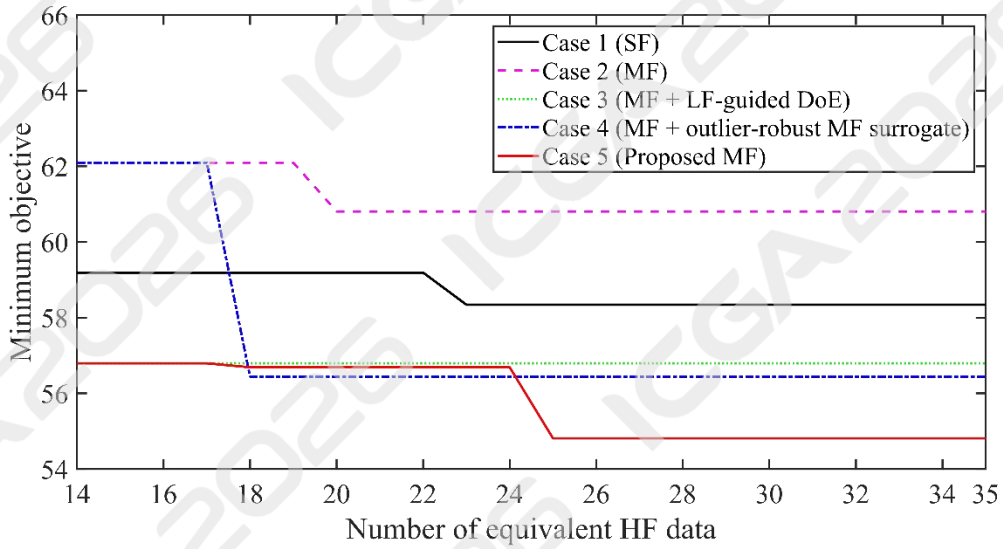
3-2. Ablation study

❖ Effect of each proposed strategy

- Equivalent HF samples: $N_{eq} = N_{HF} + N_{LF} / 15.58$ reflects the HF-to-LF time ratio, and sampling continues up to $N_{eq} = 35$.

Case	Model	LF-guided DoE	Outlier-aware BO	N_{LF} / N_{HF}
1	SF	×	×	0 / 14
2	MF	×	×	120 / 6
3	MF	O	×	120 / 6
4	MF	×	O	120 / 6
5 (Proposed)	MF	O	O	120 / 6

Configurations and initial data



Minimum objective vs. number of equivalent HF data

Proposed: favorable starting point (DoE) + fast, robust search (outlier-aware BO)

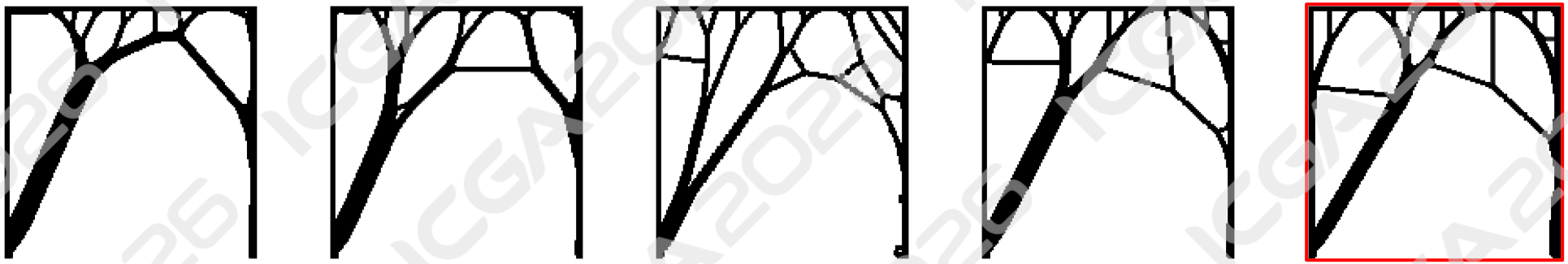
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3-2. Ablation study

❖ Optimal designs and objective values

- Diverse branch topologies confirm the presence of many local optima.
- Case 3 is trapped in its initial basin; Case 4 is limited by poor initial samples.



(a) Case 1: **58.34** (b) Case 2: **60.81** (c) Case 3: **56.79** (d) Case 4: **56.44** **(e) Case 5: 54.81**

Case	p_{ini}	p_{final}	β_{ini}	β_{final}	$move$	x_0	Obj.
1	5.90	5.66	1.00	50.00	0.12	0.10	58.34
2	4.67	4.30	1.00	32.13	0.05	0.10	60.81
3	3.17	9.92	6.65	48.13	0.11	0.29	56.79
4	3.21	8.52	1.00	50.00	0.05	0.09	56.44
5 (Proposed)	2.99	10.00	1.00	50.00	0.15	0.89	54.81

Case 5 (proposed) achieves the lowest compliance: 54.81 vs. 58.34 (SF)

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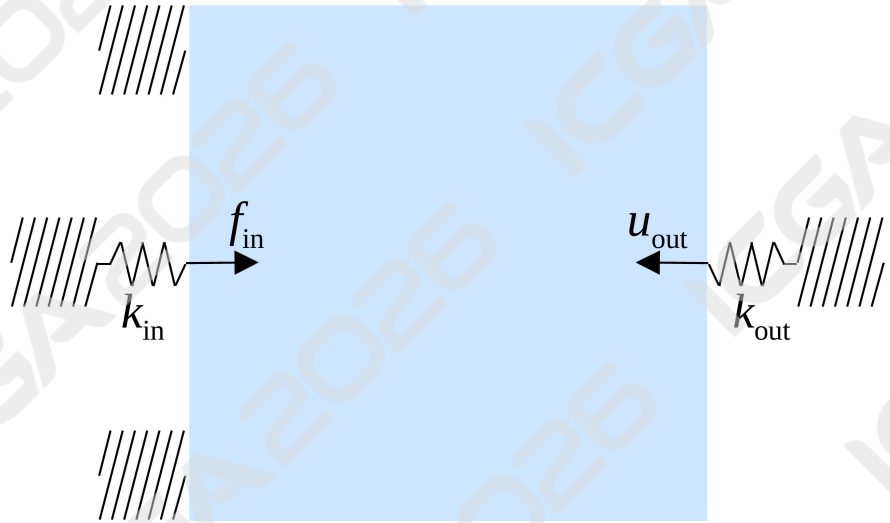
※ MCS: Monte Carlo simulation
※ HF: high-fidelity
※ LF: low-fidelity

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3-3. Compliant mechanism problem

❖ Numerical example 2: problem with numerous local optima

- The goal is to maximize the output displacement u_{out} under the input force f_{in} ($k_{\text{in}} = k_{\text{out}} = 0.1$).
- A 200 × 100 half-domain (symmetry) with a volume fraction of 0.3 and the same hyperparameters is used.
- The results are compared with SIMP at reference values and MCS with 1,000 HF samples.



Compliant mechanism problem

Method	N_{HF}	N_{LF}	N_{eq}
SIMP	1	0	1
MFTO (Proposed)	27 (6 + 21)	90	40.5
MCS	1,000	0	1,000

Number of samples (HF-to-LF time ratio: 6.66)

SIMP
Accuracy baseline:
a single run at the reference values

MCS
Efficiency baseline:
1,000 random HF runs

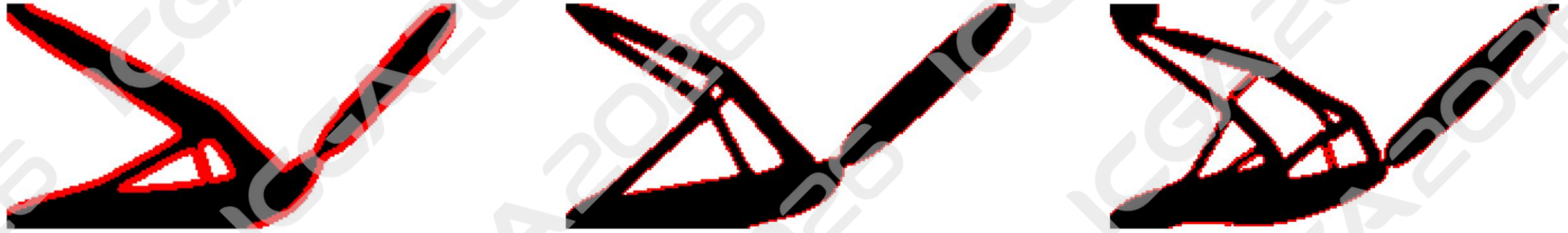
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3-3. Compliant mechanism problem

※ $|u_{out}|$: *larger is better*

❖ Optimal designs (gray regions shown in red)



(a) (b) (c)

(a) SIMP, (b) MFTO (Proposed), (c) MCS

	SIMP	MFTO (Proposed)	MCS
N_{eq}	1	40.5	1,000
Raw $\|u_{out}\|$	1.0031	1.1215	1.1251
Post-processed $\|u_{out}\|$	0.8549	**1.1128**	0.9974
Total time	≈ 433 s	≈ 6.4 h	≈ 135.9 h

−95.3% **Computation cost vs. MCS**
6.4 h vs. 135.9 h

+30.2% **Post-processed $|u_{out}|$ vs. SIMP**
1.1128 vs. 0.8549

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3-4. Advantages and limitations

❖ Discussion of the proposed method

Advantages

1. **Better optima than a single SIMP run**
   The method finds better designs than a single SIMP run with reference hyperparameters
2. **Higher accuracy than MF baselines**
   The method outperforms conventional MF surrogates via TO-tailored data generation, labeling, modeling and optimization.
3. **Higher efficiency than random-search baseline**
   The method is more efficient than the random-search baseline and conventional surrogate-based approaches.

Limitations

1. **Bounded search space**
   The global optimum may lie outside the predefined hyperparameter settings.
2. **Multiple SIMP runs required**
   The method requires multiple SIMP runs, so it is less efficient than a single SIMP run.
3. **Moderate evaluation budget needed**
   The method is most effective when tens to hundreds of SIMP evaluations are affordable.

Best suited when solution quality is prioritized under a limited HF budget

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Ⅰ. Introduction

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4. Conclusion

❖ Proposed framework

- An outlier-aware MFTO framework is proposed for hyperparameter-level TO under a limited HF budget.
- Outliers are detected, labeled and exploited throughout data generation, surrogate modeling and optimizati on.
- LF-guided DoE and an outlier-aware acquisition function concentrate HF samples in promising, feasible reg ions.

❖ Numerical results

- Frame reinforcement: the combined framework achieves the lowest compliance (54.81 vs. 58.34 for SF).
- Compliant mechanism: the method gives the best post-processed performance with about 95% less compu tation time than MCS.

❖ Future work

- Each sub-stage will be refined, and the framework will be extended to multiple LF models.
- We will extend the framework to dynamic topology optimization by addressing potentially weak LF–HF corr elations and developing correlation-aware sampling strategies.

Any questions?



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