

Highlights

Comparison of surrogate strategies for damage-aware optimization of buckling-delayed shear-link dampers with adaptive finite element validation

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- Adaptive surrogates optimize damage-aware shear-link damper geometries
- RBF interpolation ~~matches supervised ML with lower retraining~~ offers comparable accuracy to supervised ML at lower training cost
- FEM validation filters surrogate optima before accepting final designs
- Optimized devices balance window activation and frame damage control

Comparison of surrogate strategies for damage-aware optimization of buckling-delayed shear-link dampers with adaptive finite element validation

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Abstract

Buckling-delayed shear-link dampers are passive devices used in seismic-resistant structures to concentrate energy dissipation while limiting damage to the primary system. ~~Their geometric optimization~~ Optimizing their window thicknesses requires balancing high dissipative capacity with strict control of local damage. Nonlinear finite element models can reproduce their cyclic response and provide internal quantities for optimization, such as damage indicators and local distortion, but their computational cost prevents direct use within iterative optimization loops. This work proposes an adaptive surrogate-assisted optimization framework for ~~damage-aware window-thickness optimization of~~ buckling-delayed shear-link dampers ~~within five predefined geometry families~~. Experimentally calibrated nonlinear finite element models are first used to generate reference datasets for different device configurations. Supervised learning models are evaluated, with support vector regression and Gaussian process regression ~~showing high predictive accuracy~~ providing the most accurate predictions among the candidate models, motivating the use of radial basis function surrogates as a more efficient distance-based alternative. The surrogate predictions are coupled with a differential evolution algorithm through a damage-aware objective function that controls local damage while using dissipative performance as an optimization criterion. The optimized geometries are then re-evaluated with finite element simulations. If the ~~surrogate error exceeds the adopted tolerances~~ acceptance criteria are not met, the new simulation is added to the dataset and the surrogate models are retrained. The framework enables efficient damage-aware optimization of seismic energy dissipation devices.

Keywords: Buckling-delayed shear link, seismic energy dissipation, FEM validation, surrogate modelling, radial basis functions, Differential Evolution

1. Introduction

Shear-link metallic dampers are passive energy dissipation systems used in seismic-resistant structures, designed to undergo stable inelastic deformations while limiting damage to the primary system [1]. Their configuration concentrates inelastic demand in replaceable components, enabling high energy dissipation, ductile response and stable hysteretic behavior under severe cyclic loading [2, 3]. Within this family, buckling-delayed shear-link (BDSL) dampers incorporate a mechanical configuration that promotes shear-dominated behaviour while delaying local and global buckling.

The global hysteretic response of BDSL dampers can be characterized through experimental testing. However, laboratory campaigns present important limitations when addressing design optimization problems: internal state variables such as local plastic strains, stress triaxiality or damage indicators cannot be directly measured and the high cost and logistical complexity of experimental programs restrict the number of geo-

metric configurations that can be explored. These limitations become even more critical when the design objective is not only to increase global energy dissipation and maximum displacement supported by the device, but also to control where and how damage develops within the device, making systematic optimization impractical.

In this context, finite element method (FEM) simulations provide a powerful framework for generating high-fidelity datasets across a wide range of geometric configurations, making them an ideal foundation for surrogate-based optimization strategies. Advanced nonlinear FEM models can accurately reproduce experimental cyclic behaviour, including plasticity, geometric nonlinearity, contact interactions, local instability and damage evolution, while providing access to both global response quantities and local indicators governing failure mechanisms. However, their high computational cost makes their direct use within optimization loops inefficient. This limitation motivates the use of surrogate models trained on FEM-generated data, which can approximate the structural response with reduced computational effort. The use of surrogate models enables the possibility of evaluating a large number of design

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configurations, facilitating systematic optimization.

Over the past decades, FEM has been widely used to study BDSL dampers and other passive seismic energy dissipation devices, providing detailed insight into nonlinear cyclic response, stiffness degradation and local inelastic mechanisms [4, 5]. It has also supported the optimization and parametric analysis of these devices by enabling systematic exploration of geometric configurations and performance criteria under prescribed loading [6, 7]. In this context, FEM-based studies have been extensively applied to characterize the mechanical response of metallic dampers. Motamedi et al. [8] investigated accordion metallic dampers through combined experimental and numerical analyses, assessing the influence of key geometric variables on stiffness, strength and energy dissipation. Ghamari et al. [9] studied I-shaped shear links in concentrically braced frames, while Xiong et al. [10] examined replaceable steel shear links with different short-length ratios, highlighting the strong influence of geometry on cyclic performance and failure modes. Simplified analytical and semi-empirical models have also been proposed to reduce computational cost [11] and more recent simulation-based studies have further explored the role of geometric and material variables in damper performance [12].

Geometric optimization has also been extensively explored. Zhang et al. [13] proposed a Kriging-assisted framework to maximize hysteretic energy in coupling beam dampers. Farzampour et al. [14] optimized butterfly-shaped shear links by maximizing the ratio between dissipated energy and plastic strain, while Khatibinia et al. [15, 16] developed efficient strategies for U-shaped dampers using FEM and surrogate models. Shi et al. [17] introduced a non-parametric shape optimization framework for shear panel dampers and Saleh et al. [18, 19] extended this line through topology optimization of shear-link configurations. More recent contributions include the hybrid cellular automata approach by Mendoza-Cuy et al. [20] and the statistical optimization framework by Rios et al. [21].

Data-driven approaches have mainly focused on response or property prediction. Chan et al. [22] used nonlinear autoregressive exogenous (NARX) models to reproduce hysteretic behaviour. Bae et al. [23] developed models for low-cycle fatigue estimation and Almasabha et al. [24] predicted the shear strength of short steel links using ML. Elgammal et al. [25] modelled hysteretic restoring forces using data-driven approaches, while Hu et al. [26] proposed explainable ML models for the probabilistic prediction of buckling stress. Physics-informed approaches have also been explored, such as the PINN framework proposed by Hu et al. [27].

All these works demonstrate the increasing interest in applying FEM-based and data-driven approaches, as well as in combining both, to analyse, understand and optimize seismic energy dissipation devices. However, most of these studies focus either on the prediction of the hysteretic response or on maximizing energy dissipation, leaving a critical aspect insufficiently explored: the need to control local damage while maintaining adequate dissipative capacity. In practice, excessive local damage may compromise structural integrity, reduce durability and lead to premature failure, even when global energy dissipation is improved.

The present work addresses this gap through a damage-aware surrogate-assisted optimization methodology in which the objective is not only to maximize distortion or energy dissipation, but also to balance dissipative performance with damage indicators derived from FEM simulations. The proposed approach combines: (i) experimentally calibrated nonlinear FEM models used as numerical ground truth; (ii) supervised surrogate models trained to predict local damage and distortion indicators; (iii) a Differential Evolution (DE) optimizer; and (iv) an adaptive FEM validation and retraining loop.

Figure 1 summarizes the proposed workflow. The different stages of the methodology, together with the surrogate modelling, optimization strategy, validation procedure and corresponding results and conclusions, are described in the following sections.

2. Buckling-delayed shear-link damper

The BDSL dampers analysed in this work, with one representative configuration shown in Figure 2, are steel devices designed to concentrate inelastic deformation and energy dissipation in localized reduced-thickness regions, hereafter referred to as windows, while preserving the structural integrity of the surrounding frame. The damper is connected to a load-transfer system through a mechanism that allows imposed in-plane displacement while preventing axial force transmission, thereby favouring a shear-dominated response. Under cyclic loading, the windows are expected to act as the primary dissipative regions, whereas the frame ensures load transfer and global stability.

This separation of functions leads to a non-trivial design problem. Thin windows may enhance ductility and dissipative activation, but they may also promote excessive damage localization. Conversely, thicker windows may increase strength while transferring inelastic demand to the frame. Since severe frame damage may compromise the structural integrity of the device, frame damage must be penalized more strongly than window damage. At the same time, the dissipative demand should be distributed as uniformly as possible among the windows, avoiding configurations in which a single window absorbs most of the deformation while the remaining windows stay underused. Consequently, the design problem cannot be reduced to maximizing force or total dissipated energy alone, but must also control where damage develops and how the windows participate in the dissipative process.

Accordingly, the design variables considered in this work are the window thicknesses, while the frame dimensions are kept fixed:

$$\mathbf{x} = [t_{w,1}, t_{w,2}, \dots, t_{w,N_w}], \quad (1)$$

where N_w denotes the number of windows. The device width and height are identified by B and H , respectively. Five geometry families are analysed, defined by different combinations of height, width and number of windows. Due to confidentiality constraints, the main dimensions are reported in normalized form with respect to reference values, H_{ref} and B_{ref} . Figure 3

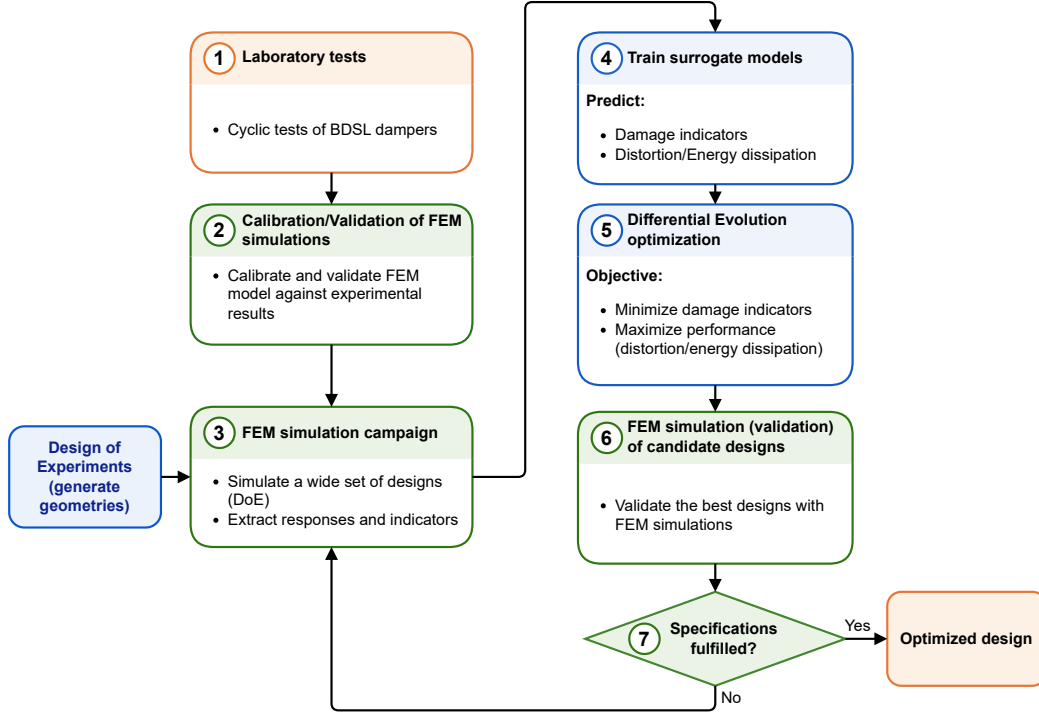


Figure 1: Flow chart of the proposed adaptive surrogate-assisted optimization framework.



Figure 2: Representative BDSL damper configuration considered in the optimization.

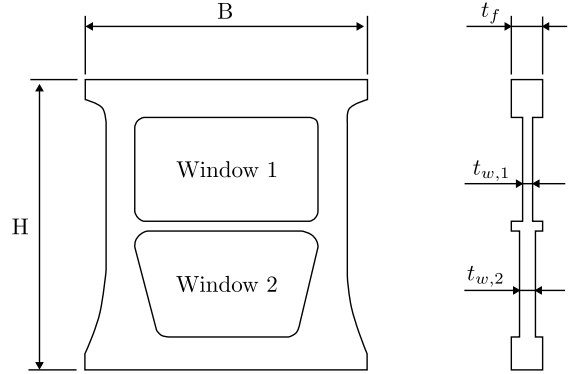


Figure 3: Geometric scheme of a representative BDSL device considered in this study.

shows the geometric scheme of one representative BDSL configuration. The example corresponds to a two-window device; throughout the paper, windows are numbered from top to bottom.

The admissible thickness ranges are defined for each geometry family according to manufacturing constraints. The main characteristics of the analysed families are summarized in Table 1. In all cases, the frame thickness is kept constant.

3. Validation of the FEM numerical model

The surrogate models developed in this work were trained using data generated from three-dimensional FEM simulations of the BDSL device under cyclic loading. The numerical model

reproduces the geometry defined in Section 2 and incorporates the boundary and loading conditions of the experimental setup. A schematic representation of the complete numerical model is shown in Figure 4. The simulations were carried out using the COMPACK code, an explicit dynamic FEM solver based on an incremental formulation for linear and nonlinear problems [28]. The model accounts for large displacements, material and geometric nonlinearities, contact interactions, support flexibility and the boundary conditions associated with the experimental configuration.

The damper is supported by a flexible base, which allows the imposed differential displacement at the support to be represented. At the top of the device, the cyclic horizontal displacement is transmitted through an actuator–connector assembly.

Table 1: Geometry families considered in the optimization and admissible window thickness ranges.

Family	H/H_{ref}	B/B_{ref}	N_w	Design variables	Thickness bounds
F_1	1.00	1.00	2	$t_{w,1}, t_{w,2}$	10–20 mm
F_2	1.00	1.17	2	$t_{w,1}, t_{w,2}$	10–20 mm
F_3	1.50	1.00	3	$t_{w,1}, t_{w,2}, t_{w,3}$	5–14 mm
F_4	1.50	1.17	3	$t_{w,1}, t_{w,2}, t_{w,3}$	5–14 mm
F_5	2.00	1.17	5	$t_{w,1}, \dots, t_{w,5}$	5–12 mm

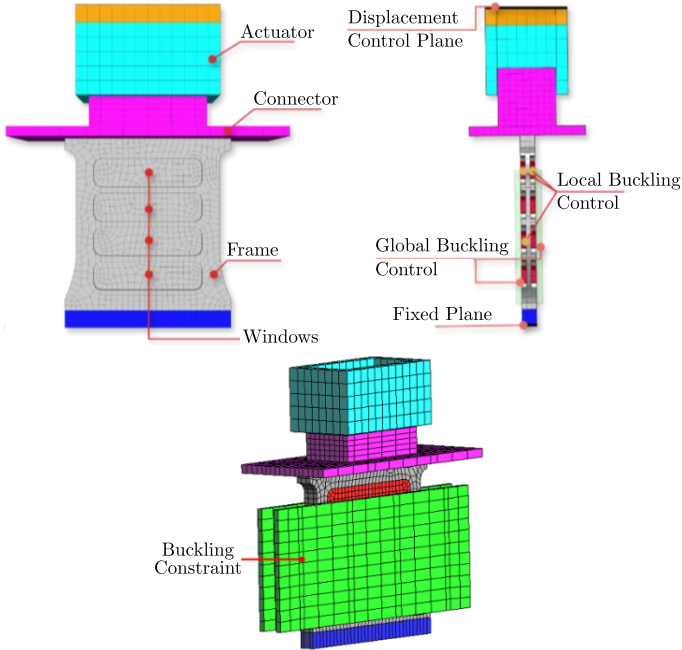


Figure 4: FEM validation model of the BDSL device: mesh discretization, main components, boundary conditions and local/global buckling control.

bly consisting of a welded connector and an actuator-like component. This assembly imposes the prescribed in-plane motion while preventing axial force transmission, thereby reproducing the shear-dominated loading condition considered in the tests. The interaction between the actuator and the connector, as well as the local and global buckling constraints introduced for the windows and the frame, are simulated through contact surfaces using a penalty-based formulation. The contact parameters were calibrated to ensure accurate displacement transmission and a stable representation of the boundary conditions.

The dissipative steel component is modelled as ASTM A36 steel, whose cyclic plastic behaviour is reproduced using the Yoshida–Uemori constitutive model [29, 30]. This formulation accounts for material nonlinearity, cyclic hardening, softening and Bauschinger-type effects under large plastic deformation. The steel component is discretized using linear eight-node hexahedral solid elements, providing a structured three-dimensional mesh suitable for extracting local stress, strain and damage-related fields. The material parameters adopted for the Yoshida–Uemori model are summarized in Table 2.

In Table 2, σ_{y0} is the initial yield stress, b is the saturated size of the backstress β , C is the hardening rate of the kinematic hardening component, m is the hardening rate of the isotropic hardening component R and of the kinematic hardening component β , B is the initial size of the bounding surface, R_{sat} is the saturated size of the isotropic hardening component and h is the expansion rate of the memory surface.

The adopted material parameters were taken from prior experimental and numerical studies on ASTM A36 steel [31], in which several specimens were tested and subsequently reproduced using the Yoshida–Uemori model. In the present work, two representative tests were used to verify the implementation of this constitutive model in COMPACK. The first one corresponds to a monotonic loading test, while the second one consists of a cyclic loading protocol with an initial cycle followed by progressively increasing displacement amplitudes until specimen failure. In both cases, the numerical response obtained with the Yoshida–Uemori formulation showed good agreement with the experimental results, as illustrated in Figure 5.

After the verification of the material model, the complete numerical model of the BDSL device was validated against three experimental tests performed according to the loading protocols defined in the ANSI/AISC 341-16 [32] and ASCE 7-22 [33] qualification standards for seismic energy dissipation devices. These protocols consist of cyclic loading histories with progres-

Table 2: Material parameters for ASTM A36 steel in the Yoshida–Uemori model.

σ_{y0} [MPa]	b [MPa]	C [MPa]	m	B [MPa]	R_{sat} [MPa]	h
255.9	194.9	338.7	7.9	277.3	196.0	0.5

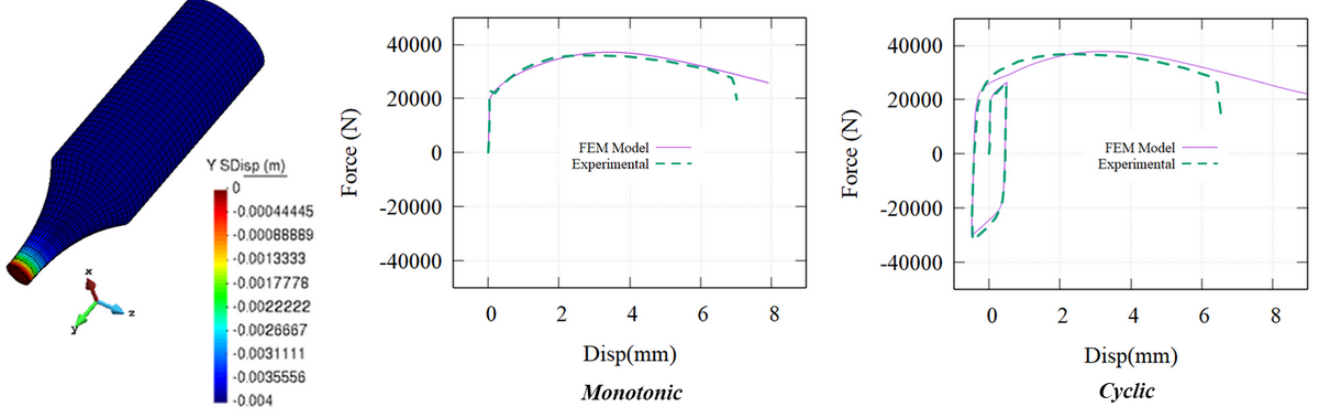


Figure 5: FEM validation of ASTM A36 steel under monotonic and cyclic loading using Yoshida–Uemori model and experimental tests.

sively increasing amplitudes. The calibration and validation procedure involved the material parameters, assembled geometry, contact definitions, support flexibility and boundary conditions of representative BDSL specimens. Further details on the numerical model and experimental campaign can be found in Ramírez et al. [34].

The validated model accurately reproduces the main global experimental responses, including the hysteretic behaviour and cumulative dissipated energy. Figure 6 compares the experimental and numerical results, confirming the suitability of the FEM model as a numerical reference for configurations beyond those experimentally tested.

4. Dataset generation and surrogate modelling

Once validated, the FEM model is used to generate the datasets required for surrogate training and optimization. The optimization strategy relies on local damage indicators in the dissipative windows and surrounding frame, together with local distortion measures associated with the activation of the dissipative mechanism.

The damage indicator adopted in this work is the Triaxial Failure Damage Map (TFDMap) [35]. This stress-triaxiality-based indicator evaluates the proximity of each material point to ductile failure by comparing, for a given triaxiality, the accumulated equivalent plastic strain with a reference failure envelope [36, 37, 38, 39]. In this study, the TFDMap is used as a post-processing damage-screening indicator, not as a constitutive fracture criterion. Its purpose is therefore not to explicitly predict crack initiation, but to compare geometrical configurations and ensure that optimized designs remain within acceptable damage levels.

4.1. Design of experiments

The FEM campaign is planned to cover an admissible range of values for the geometric parameters of each device family while ensuring a homogeneous exploration of the multidimensional space. The design variables are the window thicknesses $t_{w,i}$, whose combinations are generated through a Design of Experiments (DoE) strategy based on Latin Hypercube Sampling (LHS) optimized with the *maximin* criterion [40]. This approach provides a near-random yet space-filling distribution of samples, reducing clustering and improving the representation of the admissible range.

For each geometry family, the optimization cycle starts from an initial set of FEM simulations selected to provide reasonable coverage of the design space while keeping the computational cost as low as possible. The number of initial samples is defined according to the dimensionality of each family: 8 samples for two-window devices, 16 samples for three-window devices and 64 samples for five-window devices. In all cases, the number of samples is selected as a power of two, which facilitates the potential use of Progressive Latin Hypercube Sampling (PLHS) [41] in future iterations. This would allow the DoE to be expanded while preserving its space-filling properties and avoiding the need to repeat previously computed simulations.

To improve surrogate robustness near the admissible limits, the sampling domain is extended slightly beyond the actual optimization ranges reported in Table 1. This reduces the risk of extrapolation when evaluating candidate solutions close to the true design limits. The extended thickness ranges and the number of initial simulations for each family used in the DoE are summarized in Table 3.

For every sampled configuration, a FEM simulation is performed under a displacement-controlled cyclic loading protocol. Since the admissible deformation demand depends on the size of the device, different loading patterns are adopted accord-

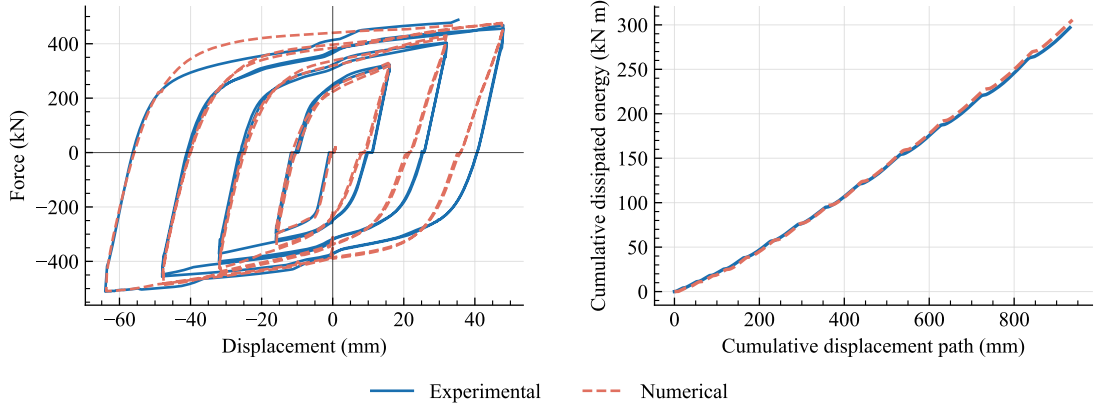


Figure 6: Experimental-numerical validation of the BDSL model: hysteretic response (left) and cumulative dissipated energy (right).

Table 3: Geometry families, window thickness ranges and number of simulations considered during the DoE generation.

Family	H/H_{ref}	B/B_{ref}	N_w	Design variables	Thickness bounds	Simulations (DoE)
F_1	1.00	1.00	2	$t_{w,1}, t_{w,2}$	8–22 mm	8
F_2	1.00	1.17	2	$t_{w,1}, t_{w,2}$	8–22 mm	8
F_3	1.50	1.00	3	$t_{w,1}, t_{w,2}, t_{w,3}$	4–16 mm	16
F_4	1.50	1.17	3	$t_{w,1}, t_{w,2}, t_{w,3}$	4–16 mm	16
F_5	2.00	1.17	5	$t_{w,1}, \dots, t_{w,5}$	4–14 mm	64

ing to the device height. As shown in Figure 7, the maximum displacement amplitude increase with the device height, consistently with the expected performance range of each geometry family.

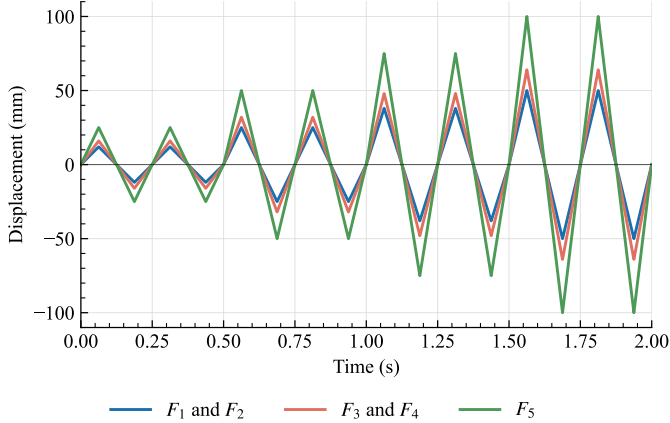


Figure 7: Displacement-controlled cyclic loading patterns adopted for the different device heights considered in the FEM campaign.

The resulting dataset stores the input variables and the structural response quantities extracted at the final time of each simulation. The target outputs include damage indicators in the windows and in the frame, together with local distortion measures associated with dissipative activation. For compactness in the optimization formulation, the aggregated TFDMaP indicator in window i is denoted by $\mathcal{D}_i$, whereas the corresponding frame indicator is denoted by $\mathcal{D}_f$. Both quantities are obtained

through a regional percentile-based aggregation, computed as the ~~average TFDMaP value of the 12 nodes with the highest values within each region. This allows to capture 98th percentile (P98) of the TFDMaP values within the corresponding region.~~ The same P98 regional statistic is used for the window distortion measure. A percentile-based regional statistic avoids defining the response through an arbitrary fixed number of nodes, while retaining the most critical damage levels while and reducing sensitivity to isolated numerical peaks.

The ~~maximum~~ local shear distortion in each window, aggregated with the same P98 regional statistic, is denoted by $\varepsilon_{xy,i}$ and is used as an indicator of the energy dissipation capacity. When included in the objective function, each window contribution is weighted according to its effective geometric volume, so that the optimization accounts for both local strain intensity and the material volume involved in the dissipation process.

4.2. Supervised ML surrogate models

This work compares several supervised surrogate models for predicting FEM-derived damage and distortion indicators. The considered models cover three families: tree-based methods, including Random Forest (RF) [42], Gradient Boosting Regression (GBR) [43] and XGBoost [44]; kernel-based methods, including Support Vector Regression (SVR) [45] and Gaussian Process Regression (GPR) [46]; and neural-network models, represented by the Multilayer Perceptron (MLP) [47, 48]. RF relies on bootstrap aggregation of decision trees, GBR and XGBoost are sequential boosting approaches, SVR and GPR exploit kernel functions to model nonlinear relationships and

MLP approximates nonlinear input–output mappings through interconnected layers.

For every geometry family, a separate regression model is trained for each target output. The input vector contains the window thicknesses of the corresponding device, while the outputs are the local distortion indicators in each window, $\varepsilon_{xy,i}$, the window damage indicators, $\mathcal{D}_i$, and the frame damage indicator, $\mathcal{D}_f$. Therefore, for a geometry family with N_w windows, $2N_w + 1$ surrogate models are trained: N_w models for window distortion, N_w models for window damage and one model for frame damage. For each output, all candidate algorithms are evaluated independently and the selected model is retained for the optimization stage.

Hyperparameters are optimized using Bayesian optimization [49], with ~~40 evaluations per model and~~ RMSE as the refit criterion. The ~~number of evaluated configurations is adapted to the dataset size, using 20 evaluations for $N \leq 20$, 30 for $21 \leq N \leq 80$ and 40 for $N > 80$.~~ The first 10 evaluations are randomly sampled to explore the search space, while the remaining ~~30 evaluations~~ are guided by the Bayesian surrogate model. This strategy provides a more efficient alternative to exhaustive grid search, particularly considering the number of geometry families, target outputs and candidate algorithms analysed. It also allows a broader exploration of continuous hyperparameter ranges. The hyperparameter search spaces considered are summarized in Appendix Appendix A.

Nested cross-validation is used to separate hyperparameter selection from generalization assessment. Hyperparameter tuning and model ranking are performed exclusively on inner folds, whereas outer folds are held out to estimate the generalization error; ~~all candidate algorithms are evaluated on the same outer splits.~~ The cross-validation strategy is adapted to the dataset size: ~~—: Leave-One-Out validation is used for $N \leq 20$, repeated four-fold five-fold cross-validation with five-three repetitions for $21 \leq N \leq 80$ and five-fold cross-validation for larger datasets.~~ For small datasets, the search spaces of tree-based models are additionally restricted to reduce overfitting.

Model selection is performed in two stages ~~using the inner cross-validation results.~~ First, for each candidate algorithm, Bayesian hyperparameter optimization is carried out using ~~cross-validated the~~ Root Mean Squared Error (RMSE) as the refit criterion. The best hyperparameter configuration is therefore the one with the lowest mean RMSE. Then, the best configurations from all candidate algorithms are compared. The model with the lowest mean RMSE defines a competitive threshold and all models with an RMSE within 5% of this value are retained. Among these competitive models, the final selection is based on the lowest relative RMSE dispersion, computed as the standard deviation of the fold-wise RMSE divided by the mean RMSE. If two models have the same dispersion, the one with the lower mean RMSE is preferred, ~~and if the dispersion cannot be estimated, the model with the lowest mean RMSE is selected.~~ This procedure, summarized in Figure 8, favours surrogates that are both accurate and stable.

Preliminary executions of the proposed workflow show that SVR or GPR always provide the highest, or second-highest, predictive accuracy for the considered datasets. These results

suggest that kernel-based models, and in particular distance-based similarity measures, are well suited to approximate the FEM response surfaces involved in this problem. This observation motivates the assessment of Radial Basis Function (RBF) interpolation [50] as a simpler and computationally efficient surrogate alternative. Although surrogate evaluation is negligible compared with FEM simulations, the training and hyperparameter optimization of complex supervised models can still become relevant when several outputs, geometry families and adaptive iterations are considered. RBF interpolation provides a non-parametric and fast-to-train alternative that can capture nonlinear response surfaces, making it attractive for low-dimensional and moderately sampled design spaces.

4.3. RBF surrogate models

The RBF surrogate is implemented using the interpolator available in the *SciPy* library [51]. For each output variable, the model is trained using the same input features employed by the supervised ML surrogates. ~~In the current implementation, a multiquadric, after standardization of the inputs. The radial basis function is adopted with zero smoothing and automatic shape-parameter selection~~ selected by inner cross-validated grid search among multiquadric, inverse multiquadric, Gaussian, linear and thin-plate spline functions. For the distance-dependent functions, the shape parameter is defined as a scaling factor times the median pairwise distance between the standardized training samples, and both the scaling factor and the smoothing parameter are included in the search.

The prediction model can be expressed as

$$\hat{y}(\mathbf{x}) = \sum_{j=1}^N \lambda_j \phi(\|\mathbf{x} - \mathbf{x}_j\|), \quad (2)$$

where $\mathbf{x}_j$ denotes the FEM-sampled geometries, λ_j represents the interpolation weights and ϕ corresponds to the selected radial basis function.

For each output variable, a final RBF surrogate is trained using all available FEM samples in the current iteration and stored for subsequent use in the optimization process. Its predictive performance is assessed through ~~Leave-One-Out validation: each FEM sample is iteratively removed from the dataset, a temporary RBF interpolant is trained with the remaining samples and the excluded sample is predicted~~ the same nested cross-validation strategy described for the supervised models, so that the RBF and the supervised alternatives are compared on identical outer splits. The resulting out-of-sample predictions are ~~then used to compute accuracy metrics in order to assess the interpolation precision and to build the out-of-fold error envelopes employed during the adaptive validation stage.~~

5. Damage-aware surrogate-assisted optimization

The proposed methodology seeks to balance damage among the dissipative windows while keeping it below a prescribed threshold. At the same time, it limits damage in the surrounding frame and promotes the highest possible energy dissipation through the activation of the windows. The ~~geometry~~

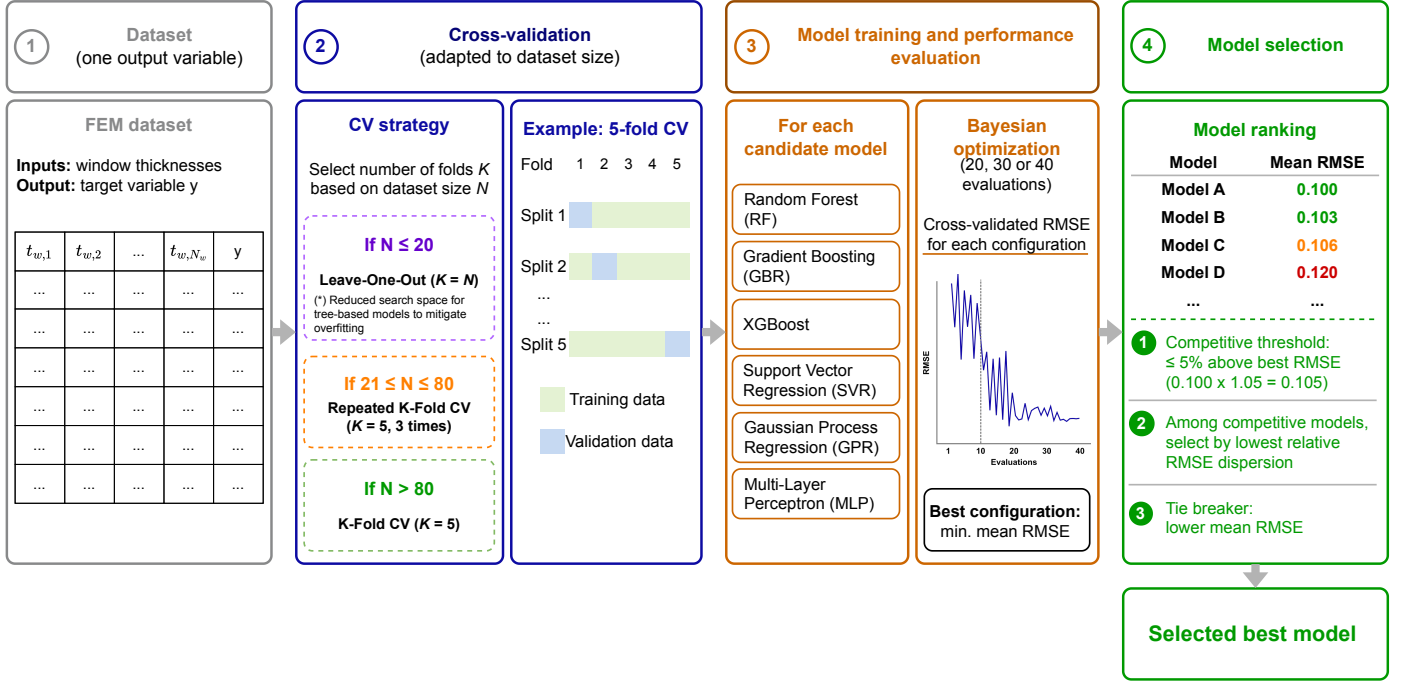


Figure 8: Workflow of the supervised surrogate training and selection strategy. For each output variable, the cross-validation strategy is adapted to the dataset size, Bayesian optimization is used to tune each candidate model and the final surrogate is selected according to RMSE accuracy and fold-wise RMSE dispersion.

window-thickness optimization is carried out using DE [52], a population-based global optimizer that does not require gradient information and is therefore suitable for nonlinear and non-convex surrogate response surfaces. In the current implementation, DE is run with a maximum of 500 iterations uses a best/1/bin strategy with a mutation factor sampled in [0.5, 1.0], a crossover probability of 0.7, a population size factor of 25, a maximum of 500 iterations and a convergence tolerance of 10^{-6} ; the initial population is generated by Latin hypercube sampling and no local polishing is applied. Each optimization stage is repeated with 30 independent runs using deterministic seeds derived from a fixed base seed. Once an optimal candidate is obtained, an adaptive FEM validation loop is applied to verify the predicted geometry before acceptance.

For each candidate geometry $\mathbf{x}$, the trained surrogate models predict the window distortions $\hat{\varepsilon}_{xy,i}$, the window damage indicators $\hat{\mathcal{D}}_i$ and the frame damage indicator $\hat{\mathcal{D}}_f$. Damage is therefore controlled in all regions of the device, but with different mechanical relevance: frame damage is penalized more severely because it may compromise the structural integrity of the damper, whereas the window damage penalties are formulated to promote comparable damage levels among windows and avoid concentrating the dissipative demand in a single region. The dissipative contribution is estimated from $\hat{\varepsilon}_{xy,i}^2$, the window thickness and the corresponding area of the window, since the energy dissipated by each window depends not only on the distortion level but also on the amount of material involved. This term is several orders of magnitude smaller than the damage penalties and is intentionally left unscaled. As a result, damage control remains the dominant criterion, while the dissipative term acts as a tie-breaker among geometries with

similar damage performance, favouring those with higher distortion and, consequently, greater energy dissipation capacity.

The implemented objective function to be minimized is

$$J(\mathbf{x}) = - \sum_{i=1}^{N_w} \hat{\varepsilon}_{xy,i}^2 t_{w,i} A_i + \sum_{i=1}^{N_w} P_w(\hat{\mathcal{D}}_i; \mathcal{D}_w^*) + P_f(\hat{\mathcal{D}}_f; \mathcal{D}_f^{\max}), \quad (3)$$

where N_w is the number of windows, $t_{w,i}$ is the thickness of window i , A_i is the corresponding area factor, $\mathcal{D}_w^*$ is the target damage level for the windows and $\mathcal{D}_f^{\max}$ is the maximum admissible frame damage threshold. The first term is negative because the optimizer minimizes J ; therefore, larger energy dissipation contributions reduce the objective value.

The window penalty is defined as

$$P_w(\hat{\mathcal{D}}_i; \mathcal{D}_w^*) = \begin{cases} (\hat{\mathcal{D}}_i - \mathcal{D}_w^*)^2, & \hat{\mathcal{D}}_i > \mathcal{D}_w^*, \\ |\hat{\mathcal{D}}_i - \mathcal{D}_w^*|, & \hat{\mathcal{D}}_i \leq \mathcal{D}_w^*. \end{cases} \quad (4)$$

This formulation penalizes values above the target quadratically, while also discouraging excessively underused windows through a linear distance to the target. As a result, the optimizer tends to balance the damage levels among windows rather than forcing all windows to remain far below the admissible level.

The frame penalty is defined as

$$P_f(\hat{\mathcal{D}}_f; \mathcal{D}_f^{\max}) = \begin{cases} (\hat{\mathcal{D}}_f - \mathcal{D}_f^{\max})^3, & \hat{\mathcal{D}}_f > \mathcal{D}_f^{\max}, \\ 0, & \hat{\mathcal{D}}_f \leq \mathcal{D}_f^{\max}. \end{cases} \quad (5)$$

The cubic penalty reflects the greater severity of frame damage compared with localized damage in a window. Since a damage value $\mathcal{D} = 100$ represents complete failure, $\mathcal{D}_f^{\max} = 90$

is adopted in the current implementation. The target window threshold is also set to $\mathcal{D}_w^* = 90$.

The surrogate-optimized geometry is not accepted directly. Instead, once an optimal geometry is identified by the surrogate-assisted optimizer, it is re-evaluated with FEM to verify that the surrogate remains accurate in the region of the design space where the optimum lies. ~~This validation step checks whether the surrogate has remained reliable in the region of the design space selected by the optimizer.~~ The Acceptance is based on FEM-confirmed physical feasibility and on the robustness of the optimizer rather than on surrogate accuracy alone. Specifically, the candidate geometry is accepted only if: (i) the ~~prediction error of all damage and distortion variables remains below the prescribed tolerance, equal to 5%~~ FEM damage indicators satisfy the prescribed physical limits in every window and in the frame; (ii) the ~~absolute error of the objective function remains within the admissible limit, set to 10;~~ and Differential Evolution result is reproducible, requiring that the performance of all independent runs is numerically indistinguishable from the best run according to a scale-aware relative criterion, with a tolerance of 10^{-3} in each optimization stage; (iii) the ~~optimized window thicknesses remain optimum~~ remains stable between consecutive ~~optimization~~ adaptive iterations, with ~~variations smaller than the 5% of the full design range.~~ If all relative changes in the stage objectives below 2%; and (iv) a conservatism check confirms that the surrogate safety margin does not materially limit the optimum. Surrogate-FEM prediction errors for the damage and distortion variables are monitored against a local out-of-fold error threshold as a diagnostic measure of surrogate fidelity, but do not by themselves determine acceptance. If the acceptance criteria are satisfied, the FEM-validated geometry is accepted as the optimized design. If at least one criterion is not satisfied, the new FEM result is added to the dataset, the surrogate models are retrained and the DE optimization is repeated. This loop, that reduces the risk of accepting a geometry that is optimal only because of surrogate extrapolation error, is summarized in Figure 9.

6. Numerical results and discussion

The supervised-learning comparison shows a ~~clear hierarchy~~ ~~predominance of kernel-based models~~ among the candidate ~~surrogate models~~ surrogates. A total of 100 output-specific ~~training-model-selection~~ problems were considered, corresponding to the $2N_w + 1$ target variables required for each geometry family and adaptive iteration. The F_1 family required two optimization iterations, whereas the remaining families required three. Across all geometry families, iterations and output variables, SVR was the most frequently selected model and also the model that most often achieved the lowest cross-validated RMSE. As summarized in Figure 10, SVR was selected in 71 cases, followed by GPR ~~, GBR, XGBoost and MLP~~ (15), GBR (10), XGBoost (2) and MLP (2), while Random Forest was not selected in any case. This ~~dominance~~ ~~predominance~~ was particularly clear for the two-window families, where only one output was assigned to a GPR model, and for the damage-related outputs, for which SVR was selected in 47 out of 57 cases. For

more complex devices, those with three and five windows, and for distortion-related outputs, the model selection became more heterogeneous, although SVR ~~still provided the best overall performance~~ remained the most frequently selected model. The RMSE-dispersion selection criterion caused the selected model to differ from the single lowest-RMSE model only in a minority of the aggregate counts; for example, GPR attained the lowest RMSE in 17 outputs but was selected in 15, whereas GBR was selected in 10 and attained the lowest RMSE in 9. These counts are descriptive statistics over model-selection tasks that are not mutually independent, because several outputs belong to the same geometry family, adaptive iteration and correlated FEM response. They are therefore reported as a descriptive summary of the comparison rather than as independent statistical evidence of superiority, and the sensitivity of the selection to the adopted 5% competitive RMSE threshold has not been assessed. From the computational point of view, SVR also offered the lowest median training times among the supervised models, whereas MLP required substantially longer training times without providing gain in accuracy.

These results indicate that kernel-based models ~~are particularly well suited to the present surrogate task.~~ SVR ~~provides~~ performed well under the adopted nested validation procedure for the datasets considered here. SVR provided the best compromise between accuracy and computational cost, while GPR ~~is was~~ the second most ~~competitive frequently selected~~ supervised strategy, especially in some higher-dimensional cases. Tree-based models ~~, although robust, are~~ were less frequently selected and MLP models ~~are were~~ not competitive in terms of computational efficiency for the dataset sizes considered ~~here~~. As mentioned in previous sections, this behaviour motivated the additional evaluation of RBF interpolation as a simpler surrogate alternative. ~~In contrast to Because the RBF and the supervised models, RBF models were trained in less than one second per output, making them especially~~ are assessed on the same outer cross-validation splits and with the same error metrics, the two strategies can be compared on a like-for-like basis at the level of each output variable. Across the analysed outputs neither strategy dominates: the selected supervised model is more accurate for some targets and the RBF surrogate for others, and both remain within the accuracy range required by the adaptive validation loop. The RBF surrogate, however, is obtained with a much smaller hyperparameter search and therefore requires substantially lower training effort, which makes it attractive for repeated surrogate updates within the adaptive optimization loop.

The predictive assessment is constrained by the small datasets available for the two-window families ($N = 8$) and the three-window families ($N = 16$). Nested cross-validation separates hyperparameter selection from generalization assessment, and the outer folds provide out-of-sample predictions together with bootstrap confidence intervals for RMSE and MAE. For datasets with $N \leq 20$ the outer loop is Leave-One-Out, so the reported errors are obtained from a single deterministic partition and their dispersion is estimated by resampling the out-of-sample predictions rather than by repeating the outer split. These results should therefore be interpreted as an assessment

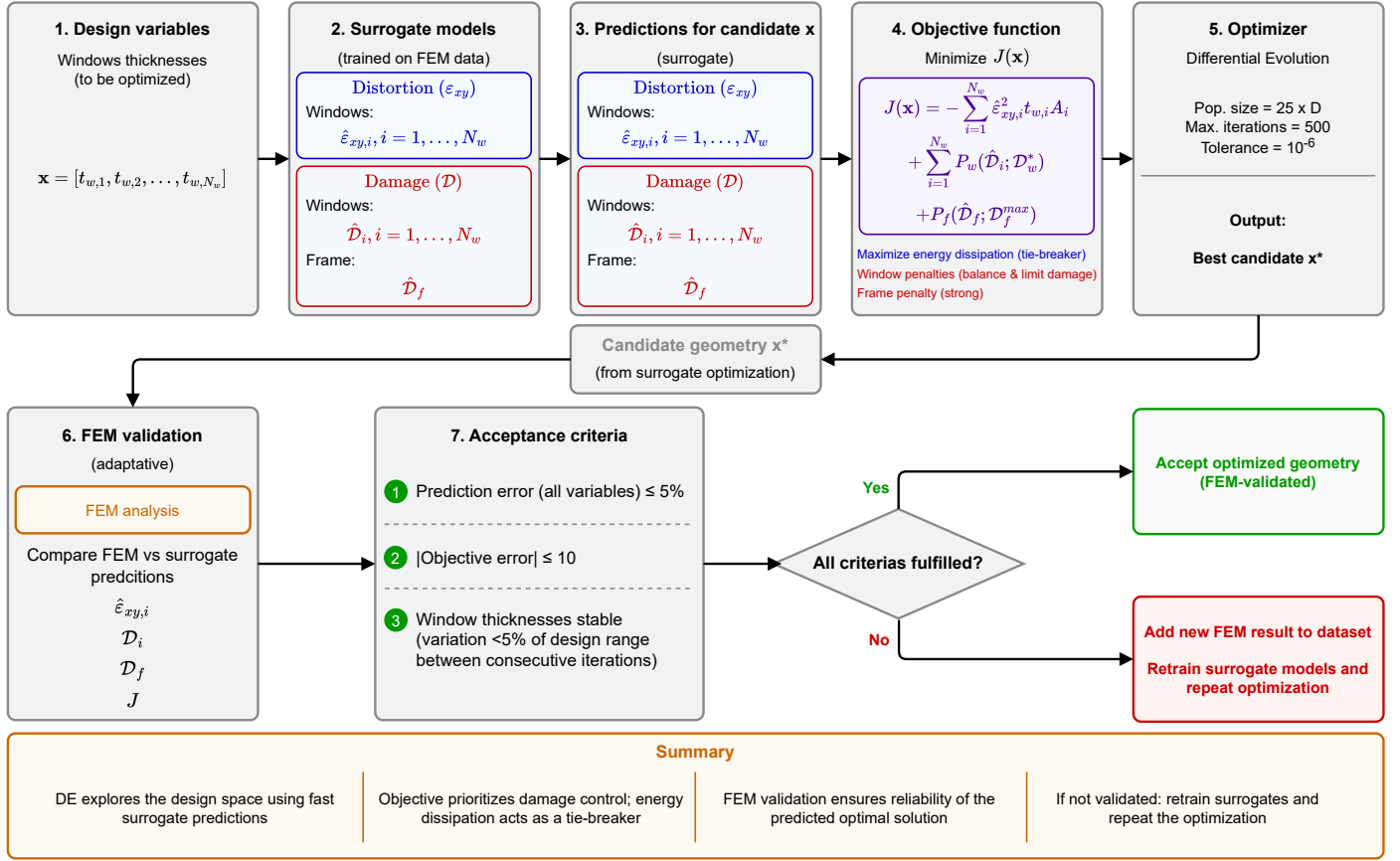


Figure 9: Surrogate-assisted optimization and FEM validation retraining loop.

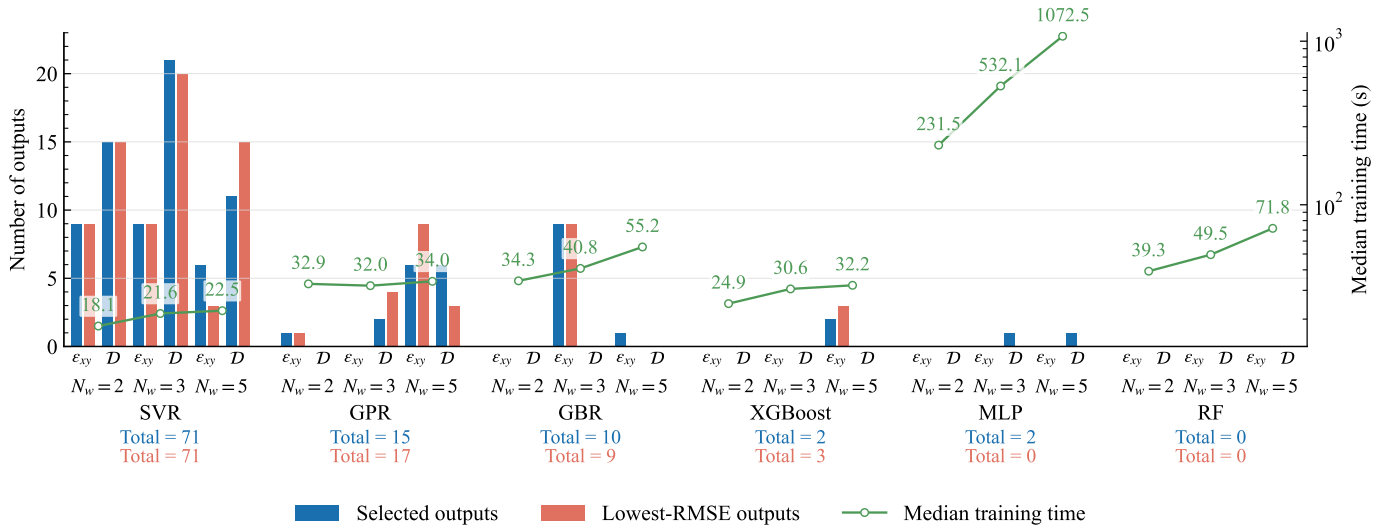


Figure 10: Summary of the supervised surrogate selection over all geometry families, adaptive iterations and target outputs. The training time corresponds to the median time required for one Bayesian hyperparameter search for a single output variable and, for visualization purposes, is in logarithmic scale.

of predictive accuracy within the sampled design domain and for the analysed geometry families, under the adopted validation procedure, rather than as a general guarantee. No independent FEM test set was retained, and the uncertainty of the accuracy estimates for the smallest datasets remains a limitation of the present comparison.

The FEM validation of the optimized geometries is summarized in Table 4, while the complete optimization results for all adaptive iterations are provided in Appendix Appendix B. For each geometry family and surrogate strategy, Table 4 reports the final accepted adaptive iteration, the optimized window thicknesses t_w^* , the surrogate-predicted objective value J_{surf} , the corresponding FEM-recomputed objective value J_{FEM} and the associated validation errors, $|e_J|$ and e_{max} . The maximum variable error, e_{max} , is defined as the largest relative error among all quantities entering the objective function, namely ε_{xyj} , $\mathcal{D}_i$ and $\mathcal{D}_f$, whereas $|e_J|$ denotes the absolute objective-function error. It should be emphasised that these errors measure the agreement between the surrogate and the FEM model at the optimized candidate; they characterise the local consistency of the surrogate in the vicinity of the optimum and are not, by themselves, a measure of global predictive accuracy over the whole design domain. The optimization required between two and three adaptive iterations depending on the geometry family and surrogate type, with most cases converging after three iterations. No systematic difference in the number of iterations was observed between RBF and supervised ML surrogates.

The final validation results show that both surrogate strategies provide FEM-consistent optimized geometries after only a few adaptive iterations. For the set of optimized candidates analysed here, RBF surrogates generally lead to lower objective-function discrepancies, with an average $|e_J|$ of 1.36, compared with 5.04 for the supervised ML surrogates. The average maximum variable error is also lower for RBF, with 1.79% compared with 2.67% for supervised ML. The RBF surrogate provides particularly accurate predictions for the two-window devices, with e_{max} below 0.3%, while remaining below 4.3% for the three- and five-window families. The supervised ML surrogates also satisfy all validation criteria provide FEM-consistent results, although larger discrepancies are observed in some cases, especially for the F_5 family, where the objective-function error reaches 9.97. These figures quantify surrogate–FEM agreement at the optimized candidates and are therefore a local validation of the accepted designs; they are not a global ranking of predictive accuracy over the design domain, for which the outer cross-validation results discussed above should be consulted.

The adaptive validation loop is essential to reach these levels of agreement. In several cases, the first surrogate-optimized candidate did not satisfy the prescribed error tolerances, particularly for the three- and five-window devices. After incorporating the additional FEM results and retraining the surrogates, the prediction errors decreased significantly. For instance, the maximum variable error of the RBF surrogate decreased from 13.70% to 1.70% in the F_3 family and from 11.44% to 2.66% in the F_5 family. A similar behaviour was observed for the supervised ML surrogates, whose final candidates also satisfied

all acceptance criteria reached a comparable level of agreement. This confirms that the adaptive loop reduces the risk of accepting geometries that appear optimal only because of surrogate prediction errors in sparsely sampled regions of the design space.

The optimized geometries obtained with RBF and supervised ML surrogates are very similar in most geometry families. In general, the differences in the optimized window thicknesses are below 0.1 mm and always below 0.2 mm, except for the F_2 family. In this case, the differences reach 0.43 mm and 1.05 mm for the first and second windows, respectively. This family also presents the largest objective-function values, indicating that the prescribed damage targets, $\mathcal{D}_i$ and $\mathcal{D}_f$, cannot be fully maintained below the desired threshold within the admissible thickness range. Consequently, the optimizer is forced to find the best compromise between damage control and dissipative activation, which may amplify the differences between surrogate predictions.

Figure 11 shows the evolution of the window thicknesses during the adaptive optimization process. In most cases, the largest adjustment occurs between the first and second iterations, while the changes between the second and third iterations are considerably smaller, indicating convergence of the proposed geometry. According to the acceptance criteria, the maximum variation in any window thickness between the last two iterations must remain below 5% of the corresponding design range. This condition is satisfied in all validated cases, with a maximum observed variation of 4.44% that the adaptive process approaches a stable optimized configuration. The progressive reduction of the thickness adjustments is consistent with the requirement that the optimum remains stable between consecutive adaptive iterations. Therefore, the adaptive process converges not only in terms of surrogate prediction accuracy, but also in terms of the optimized geometry proposed by the optimizer.

From a methodological point of view, these results highlight the trade-off between surrogate complexity, accuracy and computational efficiency. Supervised models, particularly SVR and GPR, provide high predictive accuracy and robustness competitive predictive accuracy under the adopted validation procedure, but require hyperparameter optimization and cross-validation for every output variable and adaptive iteration. RBF interpolation, in contrast, has a much lower training cost and provides very competitive final predictions once the relevant regions of the design domain have been adaptively sampled. Therefore, the comparison does not identify a universally superior surrogate strategy. Instead, it suggests that RBF interpolation is especially suitable for low- to moderate-dimensional design spaces with well-distributed FEM samples and relatively smooth input–output relationships, as occurs for the response variables analysed in this work. Supervised ML surrogates remain valuable when greater robustness is required or when the response surface is expected to involve stronger nonlinear interactions, local irregularities or higher-dimensional dependencies.

The objective-function values should also be interpreted carefully. The objective-function error measures the consis-

Table 4: Final FEM validation of the optimized geometries obtained with supervised ML and RBF surrogates.

Family	Surrogate	Iterations	t_w^* [mm]	J_{surr}	J_{FEM}	$ e_J $	e_{max} [%]
F_1	RBF	3	[12.56, 14.79]	0.00	0.41	0.41	0.29
F_1	Supervised ML	2	[12.53, 14.75]	0.00	0.08	0.08	3.14
F_2	RBF	3	[14.77, 18.95]	688.53	691.06	2.53	0.10
F_2	Supervised ML	3	[15.20, 20.00]	796.29	802.64	6.35	0.64
F_3	RBF	3	[5.81, 7.88, 8.98]	0.00	0.93	0.93	1.70
F_3	Supervised ML	3	[5.72, 7.87, 8.96]	0.00	7.47	7.47	2.85
F_4	RBF	2	[6.81, 9.02, 9.65]	0.00	1.39	1.39	4.21
F_4	Supervised ML	3	[6.84, 9.05, 9.73]	0.00	1.35	1.35	2.91
F_5	RBF	3	[5.77, 7.38, 8.37, 6.18, 5.00]	17.74	19.26	1.51	2.66
F_5	Supervised ML	3	[5.74, 7.46, 8.50, 6.37, 5.00]	16.90	26.87	9.97	3.81

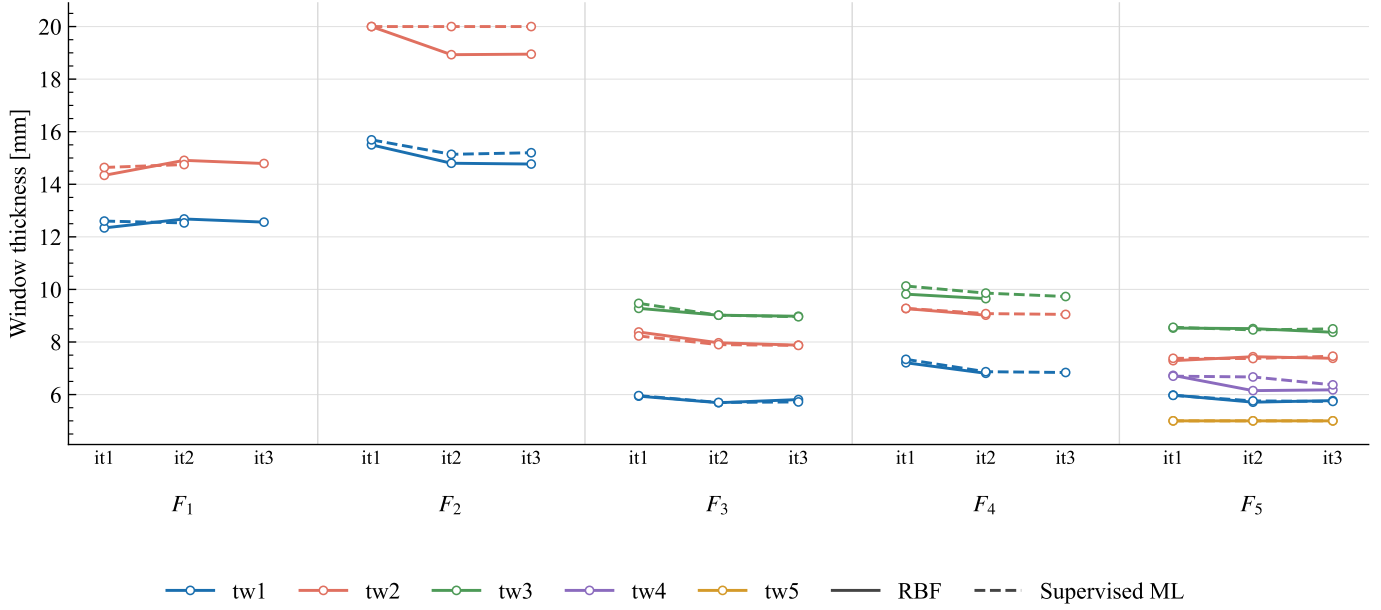


Figure 11: Evolution of the optimized window thicknesses during the adaptive optimization process.

tency between surrogate predictions and FEM validation, not whether the final objective value is necessarily close to zero. Some geometry families, such as F_2 , retain non-negligible penalty contributions because the prescribed damage targets cannot be fully achieved within the admissible design bounds. Nevertheless, the close agreement between surrogate and FEM objective values indicates that the accepted designs are not artifacts of surrogate extrapolation, but FEM-consistent optimized candidates within the explored design space.

This behaviour is illustrated in Figure 12, which shows the evolution of the RBF objective surface during the adaptive optimization process for the two-window families. The response surfaces remain relatively smooth, supporting the suitability for the two-window families considered, consistently with the good performance of RBF interpolation for this problem observed for these datasets. The evolution between adaptive iterations also shows how the surrogate surface is progressively corrected as new FEM information is incorporated near the optimized region.

7. Conclusions and future work

This work presents an adaptive surrogate-assisted optimization framework for the seismic window-thickness optimization of buckling-delayed shear-link dampers subjected to cyclic seismic loading within five predefined geometry families. The proposed methodology addresses the main limitation of direct FEM-based optimization, the high computational cost associated with repeatedly evaluating nonlinear cyclic simulations. By training surrogate models on FEM-generated datasets and validating the optimized candidates through additional FEM analyses, the optimizer can efficiently explore the design domain while remaining consistent with the mechanical response captured by the calibrated numerical model.

One of the key features of the proposed optimization framework, compared to approaches focused primarily on energy maximization, is the formulation of an objective function that takes damage into account. The aim is to prioritise local damage control in both the dissipative windows and the surrounding frame, whilst promoting a balanced contribution from all windows to the energy dissipation process. Thus, damage to the

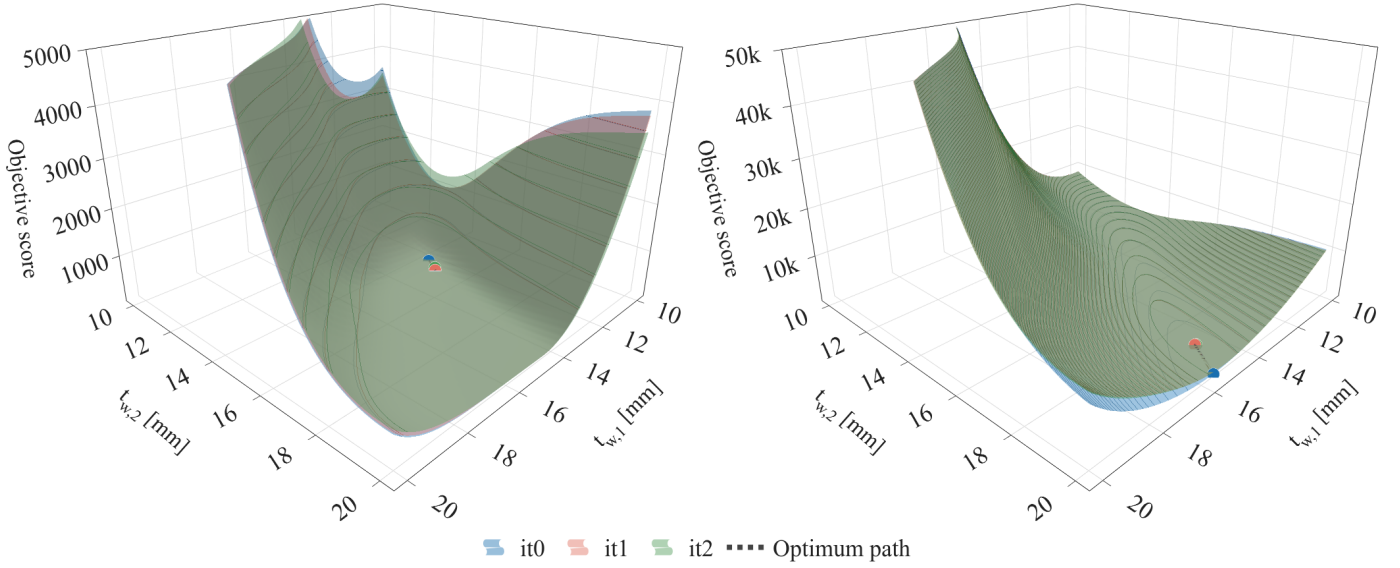


Figure 12: Evolution of the RBF objective surface during the adaptive optimization process for the two-window families. Left: F_1 . Right: F_2 .

windows is permitted and expected, as they are intended to act as dissipative regions, provided that it remains controlled and reasonably distributed; conversely, damage to the frame is penalised more severely because it can compromise the structural integrity of the damper. Therefore, rather than merely maximizing the energy dissipated, the proposed formulation favours geometries that concentrate dissipative activation in the windows, prevent excessive damage localization in a single region and protect the frame from critical damage.

A ~~comprehensive~~ comparison of surrogate strategies was performed in terms of predictive accuracy and computational efficiency. ~~The~~ For the analysed datasets, the supervised ML results showed that ~~kernel-based models, particularly SVR and GPR, were the most competitive models frequently selected, with SVR being the most frequently selected across the analysed outputs. RBF interpolation proved to be even a better alternative, due to its high efficiency: in the final adaptive iterations, it achieved validation errors outputs.~~ When evaluated on the same outer cross-validation splits, RBF interpolation provided predictive performance comparable to the supervised models for the considered low-dimensional response surfaces, while requiring a much smaller hyperparameter search and substantially lower training effort. For the optimized candidates, the RBF surrogate also achieved surrogate-FEM agreement comparable to, and in ~~most cases lower than, those several cases better than, that of the supervised ML surrogates, while requiring substantially lower training effort and no hyperparameter search.~~ This performance is attributed to the characteristics of the present problem: low to moderate-dimensional design spaces, well-distributed FEM samples and nonlinear but relatively smooth relationships between window thicknesses and response indicators. These observations are limited to the analysed geometry families and to the sampled design domain, and their reliability is lower for the smallest datasets, for which the accuracy estimates carry

larger uncertainty.

The proposed adaptive validation loop proved to be necessary and effective. Several initially optimized candidates did not satisfy the prescribed error tolerances. After incorporating the new FEM results into the training dataset and retraining the surrogates, the prediction errors decreased and ~~all final optimized geometries satisfied the acceptance criteria the optimization converged~~ after only two or three iterations. Therefore, the final designs are not accepted solely on the basis of surrogate predictions, but are explicitly verified through FEM in the region of the design space where the optimum is located.

It is also worth noting that, although the framework allows the DoE to be expanded with additional FEM simulations when the surrogate accuracy is insufficient, this was not required in the present application. The initial DoE datasets were already adequate to obtain accurate optimized designs after adaptive validation and retraining. In particular, the final geometries were obtained from only 8 initial FEM simulations for the two-window devices, 16 for the three-window devices and 64 for the five-window devices, with a maximum of three adaptive retraining iterations in all cases. This demonstrates that the proposed strategy can achieve FEM-consistent optimized designs with a limited number of simulations, making it competitive from a computational point of view.

The proposed methodology also has some limitations that should be acknowledged. First, its reliability depends on the quality of the calibrated FEM model used to generate the training data and validate the optimized designs. Second, the TFDMap is used here as a post-processing damage indicator rather than as a constitutive fracture model; therefore, the optimized configurations should be interpreted in terms of relative damage control and proximity to critical states, not as direct predictions of crack initiation. Third, only the window thicknesses are considered as design variables; although this leads to a controlled and interpretable optimization problem, it does

not exploit the full geometric flexibility of BDSL dampers. Finally, the optimized geometries should ultimately be validated experimentally before being used to establish general design recommendations.

Future work should extend the design space by including additional geometric and mechanical variables, such as window height, window spacing, frame thickness or global device proportions. This extension would increase the dimensionality and complexity of the surrogate task. In those cases, the performance of RBF interpolation should therefore be reassessed. While RBF models performed very well in the present study, their efficiency and accuracy may decrease as the input space becomes larger or the response surfaces develop stronger local nonlinearities. In such cases, supervised ML models or hybrid surrogate strategies may become more advantageous.

A complementary line of future work is the consideration of non-symmetric cyclic loading histories or recorded seismic displacement demands. The present study focuses on symmetric cyclic protocols because they provide a standardized and industry-relevant basis for the qualification of seismic energy dissipation devices, which must satisfy prescribed cyclic testing requirements before being implemented in practice. Nevertheless, earthquake-induced demands may lead to non-symmetric deformation histories in structural components. Extending the proposed framework to asymmetric cyclic protocols or representative seismic displacement histories would therefore be an interesting step towards broader performance assessment conditions.

Another future direction is the incorporation of interpretability analyses, such as SHapley Additive exPlanations [53], to quantify the influence of each geometric variable on window damage, frame damage and dissipative activation. Although such analysis lies outside the main scope of the present study, it could provide valuable insight into the design drivers governing the behaviour of BDSL dampers and support more transparent engineering decision-making. Overall, the proposed methodology establishes a scalable basis for FEM-consistent, damage-aware optimization of seismic energy dissipation devices, while leaving room for broader design variables, richer surrogate strategies and experimental validation of the optimized configurations.

Appendix A. Hyperparameter search spaces for supervised ML surrogate models

Table A.5 summarizes the hyperparameter search spaces used for the Bayesian optimization of the supervised surrogate models. The same ranges are used for kernel-based and neural-network models across all dataset sizes, whereas the search spaces of tree-based models are automatically restricted for small datasets to reduce overfitting. The cross-validation strategy is also adapted to the dataset size: Leave-One-Out validation is used for $N \leq 20$, repeated ~~four-fold~~ ~~five-fold~~ cross-validation with ~~five~~ ~~three~~ repetitions for $21 \leq N \leq 80$ and five-fold cross-validation for larger datasets.

Appendix B. Summary of optimization results

This appendix summarizes the surrogate-predicted optimized configurations, the corresponding FEM validation values and the associated errors for all adaptive iterations. The source “Surr.” denotes the values predicted by the surrogate model during the optimization, whereas “FEM” denotes the values re-computed with the numerical model. Error rows report the relative error for the response variables and the absolute error for the objective function.

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Data availability

Due to confidentiality constraints associated with the industrial device geometries, the data associated with this study are available from the corresponding author upon reasonable request.

Declaration of generative AI and AI-assisted technologies in the manuscript preparation process

During the preparation of this work the authors used OpenAI Codex to assist with LaTeX template conversion and manuscript formatting. After using this tool, the authors reviewed and edited the content as needed and take full responsibility for the content of the article.

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Table A.5: Hyperparameter search spaces used for Bayesian optimization of the supervised surrogate models.

Model	Preprocessing / kernel	Hyperparameter	Search space
RF	–	$n_{\text{estimators}}$	S/M/L: [200, 800]/[300, 1200]/[200, 2000]
		max depth	S/M/L: [1, 4]/[2, 10]/[5, 40]
		min samples split	S/M/L: [2, 8]/[2, 10]/[2, 10]
		min samples leaf	S/M/L: [2, 4]/[1, 6]/[1, 6]
		max features	S/M/L: [0.5, 1.0]/[0.5, 1.0]/[0.5, 1.0]
GBR	–	$n_{\text{estimators}}$	S/M/L: [200, 1500]/[300, 2500]/[200, 3000]
		learning rate	S/M/L: [10^{-2} , 8×10^{-2}]/[10^{-3} , 10^{-1}]/[10^{-3} , 10^{-1}]
		max depth	S/M/L: [1, 3]/[1, 4]/[2, 6]
		subsample	S/M/L: [0.7, 0.9]/[0.6, 1.0]/[0.6, 1.0]
		max features	S/M/L: [0.6, 1.0]/[0.5, 1.0]/[0.5, 1.0]
XGBoost	–	$n_{\text{estimators}}$	S/M/L: [200, 1200]/[300, 1600]/[200, 2000]
		max depth	S/M/L: [1, 4]/[2, 6]/[3, 8]
		learning rate	S/M/L: [10^{-2} , 0.2]/[10^{-3} , 0.3]/[10^{-3} , 0.3]
		subsample	S/M/L: [0.7, 0.95]/[0.6, 1.0]/[0.6, 1.0]
		colsample by tree	S/M/L: [0.7, 1.0]/[0.6, 1.0]/[0.6, 1.0]
SVR	StandardScaler + RBF kernel	C	[10^0 , 10^4]
		γ	[10^{-4} , 10^{-1}]
		ϵ	[10^{-4} , 10^{-1}]
GPR	StandardScaler	kernel	{RBF, Matern $_{3/2}$, Matern $_{5/2}$, RQ}
		amplitude	[10^{-2} , 10^2]
		length scale	[10^{-2} , 10^2]
		α_{RQ}	[10^{-2} , 10^2]
		noise	[10^{-12} , 10^{-4}]
MLP	StandardScaler	restarts	[1, 10]
		hidden layers	[1, 5]
		neurons per layer	[64, 512]
		activation	{ReLU, tanh}
		α	[10^{-5} , 10^{-2}]
		initial learning rate	[10^{-4} , 10^{-2}]

Note: For tree-based models, the hyperparameter ranges are adapted to the dataset size: S denotes small sample $N \leq 20$, M denotes medium sample $21 \leq N \leq 80$ and L denotes large sample $N > 80$. For the remaining models, the same search spaces are used for all dataset sizes.

Table B.6: Optimization results for the F_1 family using Supervised ML surrogates.

Iter.	Source	t_w [mm]	ϵ_{xy}	$\mathcal{D}_w$	$\mathcal{D}_f$	J
1	Surr.	[12.60, 14.64]	[0.05048, 0.06183]	[90.00, 90.00]	89.65	0.00
	FEM	[12.60, 14.64]	[0.04501, 0.0616]	[88.25, 91.19]	87.17	3.16
	Error	–	[12.15%, 0.37%]	[1.99%, 1.30%]	2.84%	3.16
2	Surr.	[12.53, 14.75]	[0.04602, 0.06061]	[90.00, 90.00]	89.32	0.00
	FEM	[12.53, 14.75]	[0.04555, 0.06053]	[89.95, 90.18]	86.61	0.07947
	Error	–	[1.03%, 0.12%]	[0.05%, 0.20%]	3.14%	0.0795

Table B.7: Optimization results for the F_2 family using Supervised ML surrogates.

Iter.	Source	t_w [mm]	ϵ_{xy}	$\mathcal{D}_w$	$\mathcal{D}_f$	J
1	Surr.	[15.69, 20.00]	[0.05065, 0.04732]	[105.29, 72.51]	96.62	541.95
	FEM	[15.69, 20.00]	[0.05127, 0.04603]	[103.51, 73.24]	99.21	980.46
	Error	–	[1.21%, 2.80%]	[1.72%, 0.99%]	2.61%	438.51
2	Surr.	[15.14, 20.00]	[0.05444, 0.04442]	[110.55, 71.35]	97.30	830.19
	FEM	[15.14, 20.00]	[0.05413, 0.04418]	[110.40, 71.84]	97.12	795.11
	Error	–	[0.58%, 0.53%]	[0.14%, 0.68%]	0.19%	35.08
3	Surr.	[15.20, 20.00]	[0.05398, 0.0441]	[109.73, 71.61]	97.30	796.29
	FEM	[15.20, 20.00]	[0.05379, 0.04439]	[109.65, 72.03]	97.36	802.64
	Error	–	[0.36%, 0.64%]	[0.07%, 0.59%]	0.06%	6.35

Table B.8: Optimization results for the F_3 family using Supervised ML surrogates.

Iter.	Source	$\mathbf{t}_w$ [mm]	ϵ_{xy}	$\mathcal{D}_w$	$\mathcal{D}_f$	J
1	Surr.	[5.96, 8.23, 9.47]	[0.05164, 0.04547, 0.04887]	[90.00, 90.00, 90.00]	71.00	0.00
	FEM	[5.96, 8.23, 9.47]	[0.04637, 0.04648, 0.05136]	[89.20, 85.22, 83.96]	68.08	11.62
	Error	–	[11.37%, 2.18%, 4.85%]	[0.90%, 5.61%, 7.19%]	4.28%	11.62
2	Surr.	[5.70, 7.90, 9.02]	[0.04801, 0.0478, 0.0493]	[90.00, 90.00, 90.00]	71.22	0.00
	FEM	[5.70, 7.90, 9.02]	[0.04906, 0.04815, 0.05333]	[93.70, 89.65, 88.89]	68.18	15.15
	Error	–	[2.14%, 0.73%, 7.55%]	[3.95%, 0.39%, 1.25%]	4.46%	15.15
3	Surr.	[5.72, 7.87, 8.96]	[0.04862, 0.04822, 0.05305]	[90.00, 90.00, 90.00]	68.58	0.00
	FEM	[5.72, 7.87, 8.96]	[0.04846, 0.04798, 0.05389]	[92.64, 89.69, 89.81]	68.52	7.47
	Error	–	[0.32%, 0.50%, 1.57%]	[2.85%, 0.34%, 0.21%]	0.09%	7.47

Table B.9: Optimization results for the F_4 family using Supervised ML surrogates.

Iter.	Source	$\mathbf{t}_w$ [mm]	ϵ_{xy}	$\mathcal{D}_w$	$\mathcal{D}_f$	J
1	Surr.	[7.34, 9.28, 10.13]	[0.03217, 0.03708, 0.05097]	[90.00, 90.00, 90.00]	71.57	0.00
	FEM	[7.34, 9.28, 10.13]	[0.03834, 0.04702, 0.05298]	[80.76, 86.78, 87.08]	69.66	15.38
	Error	–	[16.10%, 21.13%, 3.79%]	[11.44%, 3.71%, 3.35%]	2.75%	15.38
2	Surr.	[6.87, 9.08, 9.86]	[0.03612, 0.05013, 0.05362]	[90.00, 90.00, 90.00]	68.42	0.00
	FEM	[6.87, 9.08, 9.86]	[0.04277, 0.04322, 0.05375]	[90.40, 89.46, 88.14]	68.49	2.56
	Error	–	[15.56%, 15.99%, 0.24%]	[0.44%, 0.60%, 2.11%]	0.10%	2.56
3	Surr.	[6.84, 9.05, 9.73]	[0.04169, 0.04354, 0.05319]	[90.00, 90.00, 90.00]	68.81	0.00
	FEM	[6.84, 9.05, 9.73]	[0.04271, 0.04299, 0.05478]	[90.36, 89.19, 89.59]	68.94	1.35
	Error	–	[2.40%, 1.27%, 2.91%]	[0.40%, 0.90%, 0.46%]	0.19%	1.35

Table B.10: Optimization results for the F_5 family using Supervised ML surrogates.

Iter.	Source	$\mathbf{t}_w$ [mm]	ϵ_{xy}	$\mathcal{D}_w$	$\mathcal{D}_f$	J
1	Surr.	[5.97, 7.38, 8.56, 6.70, 5.00]	[0.05963, 0.05258, 0.06459, 0.06971, 0.05512]	[90.00, 90.00, 90.00, 90.00, 79.42]	74.65	10.58
	FEM	[5.97, 7.38, 8.56, 6.70, 5.00]	[0.05635, 0.05188, 0.05966, 0.07124, 0.05824]	[84.95, 90.65, 87.91, 81.06, 74.18]	79.15	32.33
	Error	–	[5.83%, 1.36%, 8.27%, 2.14%, 5.35%]	[5.94%, 0.72%, 2.38%, 11.03%, 7.07%]	5.69%	21.74
2	Surr.	[5.76, 7.37, 8.46, 6.67, 5.00]	[0.0615, 0.05313, 0.06014, 0.07067, 0.05734]	[90.00, 90.00, 90.00, 90.00, 73.04]	74.85	16.96
	FEM	[5.76, 7.37, 8.46, 6.67, 5.00]	[0.06398, 0.05679, 0.06492, 0.07844, 0.06236]	[95.56, 95.92, 92.86, 85.17, 71.37]	75.19	97.55
	Error	–	[3.88%, 6.45%, 7.36%, 9.90%, 8.05%]	[5.81%, 6.17%, 3.08%, 5.67%, 2.34%]	0.45%	80.59
3	Surr.	[5.74, 7.46, 8.50, 6.37, 5.00]	[0.06117, 0.05325, 0.0609, 0.07548, 0.05962]	[90.00, 90.00, 90.00, 90.00, 73.10]	75.62	16.90
	FEM	[5.74, 7.46, 8.50, 6.37, 5.00]	[0.06082, 0.05335, 0.05924, 0.07453, 0.05842]	[91.93, 89.75, 87.52, 86.70, 72.88]	78.19	26.87
	Error	–	[0.59%, 0.18%, 2.80%, 1.28%, 2.06%]	[2.10%, 0.28%, 2.83%, 3.81%, 0.30%]	3.29%	9.97

Table B.11: Optimization results for the F_1 family using RBF surrogates.

Iter.	Source	$\mathbf{t}_w$ [mm]	ϵ_{xy}	$\mathcal{D}_w$	$\mathcal{D}_f$	J
1	Surr.	[12.34, 14.34]	[0.04755, 0.06219]	[90.00, 90.00]	88.74	0.00
	FEM	[12.34, 14.34]	[0.04612, 0.06351]	[91.00, 94.60]	87.68	22.15
	Error	–	[3.12%, 2.07%]	[1.10%, 4.86%]	1.20%	22.15
2	Surr.	[12.68, 14.91]	[0.04531, 0.06034]	[90.00, 90.00]	87.53	0.00
	FEM	[12.68, 14.91]	[0.04499, 0.0598]	[88.74, 88.84]	86.81	2.42
	Error	–	[0.73%, 0.91%]	[1.42%, 1.31%]	0.83%	2.42
3	Surr.	[12.56, 14.79]	[0.04553, 0.06042]	[90.00, 90.00]	86.88	0.00
	FEM	[12.56, 14.79]	[0.04544, 0.06033]	[89.75, 89.84]	86.63	0.40514
	Error	–	[0.19%, 0.15%]	[0.28%, 0.18%]	0.29%	0.4051

Table B.12: Optimization results for the F_2 family using RBF surrogates.

Iter.	Source	$\mathbf{t}_w$ [mm]	ϵ_{xy}	$\mathcal{D}_w$	$\mathcal{D}_f$	J
1	Surr.	[15.50, 20.00]	[0.05243, 0.04593]	[105.09, 73.10]	96.41	507.38
	FEM	[15.50, 20.00]	[0.05211, 0.0454]	[105.82, 72.74]	98.50	880.86
	Error	–	[0.60%, 1.16%]	[0.69%, 0.50%]	2.12%	373.48
2	Surr.	[14.80, 18.93]	[0.05458, 0.04902]	[109.57, 78.18]	96.74	700.74
	FEM	[14.80, 18.93]	[0.05377, 0.04931]	[109.14, 78.71]	96.78	689.16
	Error	–	[1.52%, 0.59%]	[0.39%, 0.67%]	0.04%	11.58
3	Surr.	[14.77, 18.95]	[0.05395, 0.04908]	[109.61, 78.49]	96.64	688.53
	FEM	[14.77, 18.95]	[0.054, 0.04906]	[109.69, 78.51]	96.63	691.06
	Error	–	[0.10%, 0.05%]	[0.07%, 0.03%]	0.00%	2.53

Table B.13: Optimization results for the F_3 family using RBF surrogates.

Iter.	Source	t_w [mm]	ϵ_{xy}	$\mathcal{D}_w$	$\mathcal{D}_f$	J
1	Surr.	[5.94, 8.38, 9.28]	[0.04571, 0.05098, 0.05057]	[90.00, 90.00, 90.00]	71.81	0.00
	FEM	[5.94, 8.38, 9.28]	[0.04632, 0.04484, 0.05324]	[89.24, 82.01, 85.72]	69.82	13.04
	Error	–	[1.32%, 13.70%, 5.00%]	[0.86%, 9.75%, 5.00%]	2.85%	13.04
2	Surr.	[5.69, 7.97, 9.02]	[0.04677, 0.04855, 0.05551]	[90.00, 90.00, 90.00]	70.49	0.00
	FEM	[5.69, 7.97, 9.02]	[0.04928, 0.04787, 0.05344]	[94.17, 88.58, 88.69]	68.47	20.11
	Error	–	[5.09%, 1.42%, 3.86%]	[4.43%, 1.60%, 1.47%]	2.95%	20.11
3	Surr.	[5.81, 7.88, 8.98]	[0.04722, 0.04867, 0.05416]	[90.00, 90.00, 90.00]	69.17	0.00
	FEM	[5.81, 7.88, 8.98]	[0.04703, 0.04785, 0.05415]	[90.02, 89.07, 90.02]	68.85	0.93372
	Error	–	[0.42%, 1.70%, 0.01%]	[0.02%, 1.05%, 0.02%]	0.46%	0.9337

Table B.14: Optimization results for the F_4 family using RBF surrogates.

Iter.	Source	t_w [mm]	ϵ_{xy}	$\mathcal{D}_w$	$\mathcal{D}_f$	J
1	Surr.	[7.21, 9.27, 9.82]	[0.04351, 0.04034, 0.05378]	[90.00, 90.00, 90.00]	71.35	0.00
	FEM	[7.21, 9.27, 9.82]	[0.03892, 0.04601, 0.05525]	[82.20, 85.06, 90.33]	70.86	12.85
	Error	–	[11.80%, 12.31%, 2.66%]	[9.49%, 5.80%, 0.37%]	0.69%	12.85
2	Surr.	[6.81, 9.02, 9.65]	[0.0419, 0.04824, 0.05385]	[90.00, 90.00, 90.00]	69.63	0.00
	FEM	[6.81, 9.02, 9.65]	[0.04228, 0.04629, 0.05421]	[90.55, 89.06, 90.38]	69.09	1.39
	Error	–	[0.92%, 4.21%, 0.66%]	[0.61%, 1.05%, 0.42%]	0.78%	1.39

Table B.15: Optimization results for the F_5 family using RBF surrogates.

Iter.	Source	t_w [mm]	ϵ_{xy}	$\mathcal{D}_w$	$\mathcal{D}_f$	J
1	Surr.	[5.98, 7.29, 8.53, 6.73, 5.00]	[0.06013, 0.05438, 0.05386, 0.06869, 0.05284]	[90.00, 90.00, 90.00, 90.00, 74.98]	70.51	15.02
	FEM	[5.98, 7.29, 8.53, 6.73, 5.00]	[0.05632, 0.0526, 0.05986, 0.07083, 0.05884]	[84.59, 92.60, 89.02, 80.76, 73.89]	78.89	38.48
	Error	–	[6.77%, 3.39%, 10.02%, 3.02%, 10.19%]	[6.40%, 2.80%, 1.10%, 11.44%, 1.48%]	10.62%	23.46
2	Surr.	[5.71, 7.44, 8.51, 6.15, 5.00]	[0.05915, 0.05193, 0.06105, 0.07748, 0.05922]	[90.00, 90.00, 90.00, 90.00, 73.32]	80.01	16.68
	FEM	[5.71, 7.44, 8.51, 6.15, 5.00]	[0.05934, 0.05266, 0.05789, 0.07678, 0.05857]	[92.17, 89.57, 86.36, 90.05, 72.42]	77.82	26.36
	Error	–	[0.32%, 1.38%, 5.47%, 0.91%, 1.11%]	[2.36%, 0.47%, 4.21%, 0.06%, 1.25%]	2.81%	9.69
3	Surr.	[5.77, 7.38, 8.37, 6.18, 5.00]	[0.05805, 0.05275, 0.05965, 0.07628, 0.05832]	[90.00, 90.00, 90.00, 90.00, 72.26]	77.60	17.74
	FEM	[5.77, 7.38, 8.37, 6.18, 5.00]	[0.05914, 0.05314, 0.05986, 0.07616, 0.05681]	[89.36, 89.65, 89.64, 90.73, 72.63]	77.89	19.26
	Error	–	[1.84%, 0.73%, 0.34%, 0.14%, 2.66%]	[0.72%, 0.39%, 0.41%, 0.80%, 0.51%]	0.37%	1.51

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