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A CASCADE PHYSICS-INFORMED NEURAL NETWORK SURROGATE FOR MULTI-PARAMETRIC STRUCTURAL SIMULATION OF STEEL BEAMS UNDER ELASTO-PLASTIC DEFORMATION

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Abstract. In modern structural mechanics, the use of repetitive optimization cycles for computational models of spatial structures of buildings requires significant computational resources. Traditional Finite Element Method (FEM) analysis provides high accuracy but is prohibitively slow for iterative optimization, while fast analytical solutions often lack the necessary precision, particularly beyond the elastic material behavior of the structures. This paper proposes a surrogate neural network model based on Physics-Informed Neural Networks (PINNs) for the instantaneous prediction of deformations and stresses in steel I-beams. The model accounts for a 33-dimensional parametric space encompassing geometry, physical material properties, 6-DOF end loads, and distributed loads. It is founded on a kinematic decomposition approach and a four-stage cascade architecture (Pre-Filter, Yield Classifier, Skeleton PINN, and Flesh PINN). By employing the Halton sequence and an Active Learning mechanism to generate a database (>50,000 samples) with extremum filtering based on a relative deflection criterion of $L/50$, the model demonstrates high engineering accuracy: the Median Absolute Error (MedAE) of deflection is 0.672 mm, with the maximum error for the vast majority of complex nonlinear problems (80–90% of the sample) not exceeding 1.5 mm. Stresses are predicted with a median error of 1.99 MPa. The implementation of Uncertainty Quantification mechanisms in a “Safe Mode”, combined with physical heuristics (von Mises stress control), minimizes the proportion of undetected critical states (False Negatives) to 0.9%. This ensures strictly conservative model behavior while maintaining a high inference speed (computation time on the benchmark system was ~ 156 ms), which surpasses the speed of traditional FEM by several orders of magnitude. Furthermore, the developed approach enables the efficient integration of the surrogate model into iterative generative design and topology optimization cycles of building frameworks

Keywords: surrogate modeling; structural mechanics; Finite Element Method; Physics-Informed Neural Networks (PINN); Active Learning.

INTRODUCTION

The development of generative design of buildings and topology optimization methods creates new challenges regarding the computational speed of structural mechanics software [1–3]. The search for a rational mass distribution in multi-element spatial frameworks requires tens of thousands of stress-strain state computation iterations [17].

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Traditional analysis based on the Finite Element Method (FEM), capable of reliably modeling warping effects and elasto-plastic material behavior of structures, turns into a critical computational bottleneck.

Conversely, analytical solutions lose their validity beyond the elastic stage of structural behavior and under the influence of complex spatial loading.

The research hypothesis is predicated on overcoming this trade-off by replacing direct numerical integration with the inference of deep neural networks. The objective of this study is the development of a high-dimensional cascade Physics-Informed Neural Network (PINN) surrogate capable of functioning as a universal computational "super-element". Such a model must instantaneously approximate the response of a steel beam to arbitrary six-component loading within a 33-dimensional parametric space of physical and geometric characteristics [8].

STRUCTURAL PROBLEM FORMULATION

A modern spatial structure of a building is typically considered a discrete assembly of multiple interacting beam elements (Fig. 1). To ensure algorithmic variability, the computational model must accept an arbitrary combination of profile geometry, physical constants of steel (modulus of elasticity, yield strength), end forces, and spatial distributed loads as its input vector.

Given the specificities of the Serviceability Limit State (SLS) [4], the domain of the objective function was deliberately restricted to a relative deflection limit of $L/50$. This threshold was established to guarantee the inclusion of deep geometric and physical nonlinearity zones, which simultaneously allowed the exclusion of total collapse states that hold no practical value for operational calculations. All configurations resulting in the exceedance of this threshold or inducing singular phenomena of bifurcation buckling were classified as *a priori* inadmissible. Mathematically, buckling represents a bifurcation point where a single load vector corresponds to multiple equiprobable buckling modes (e.g., buckling in opposite directions or mutually perpendicular planes). A neural network solving a regression problem tends to find their arithmetic mean (an ideal straight line), generating an enormous error. Therefore, filtering such states is a mathematical necessity to avoid discontinuous functions. Their removal from the baseline regression dataset stabilized the gradients during the optimization of the neural network weights and focused the model's capacity on the operational elasto-plastic behavior zone.

PARAMETRIC SPACE FORMULATION AND ACTIVE LEARNING

The high dimensionality of the parametric space (33 independent variables) posed a challenge for efficient Design of Experiments (DoE). The application of classical methods,

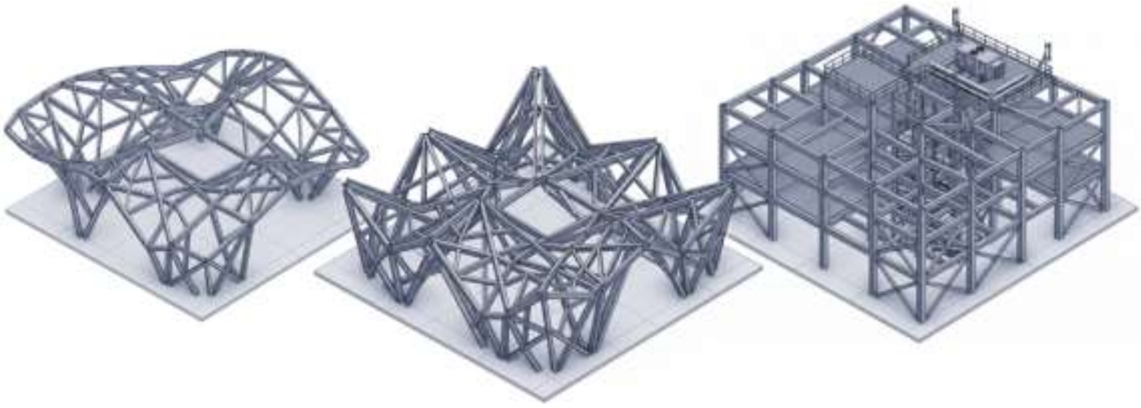

Fig. 1. Examples of spatial steel structures composed of I-beams subjected to parametric optimization.
Рис. 1. Приклади просторових конструкцій на основі сталевих двотаврових балок, до яких застосовується метод параметричної оптимізації

particularly uniform sampling via Latin Hypercube Sampling (LHS), was rejected due to the necessity of *a priori* fixation of the total dataset volume, which precluded iterative fine-tuning [16]. Instead, generation was initialized using the quasi-random Halton sequence. To ensure representativeness, data synthesis occurred under four controlled scenarios: gravitational bending, in-plane buckling, combined compression and bending, and complex spatial resistance (the block diagram of the data generation pipeline is shown in Fig. 2).

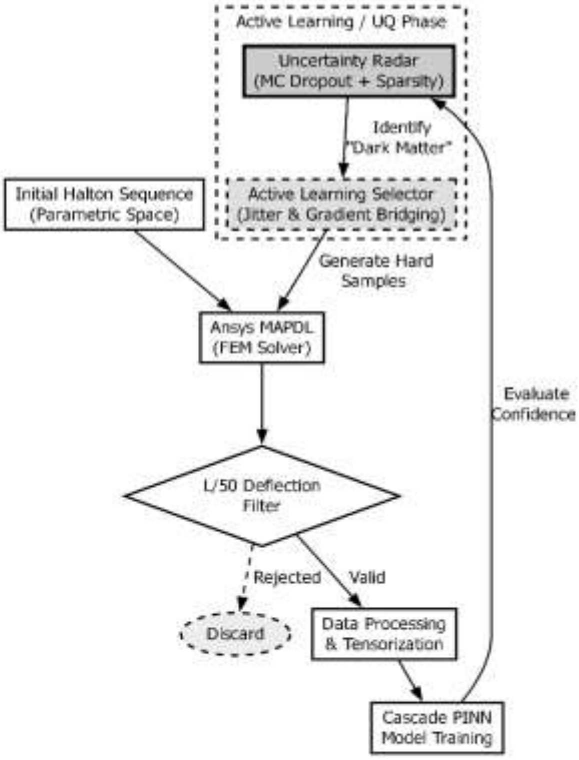

Fig. 2. Active Learning Data Generation Pipeline
Рис. 2. Конвеєр генерації даних із застосуванням активного навчання

However, intermediate training stages on volumes of up to 15,000 samples revealed a stagnation of the loss function: a distinct "glass ceiling" of accuracy was observed, where the absolute error of the deformed beam axis did not fall below 6.5 mm. Blind, extensive augmentation of the database proved ineffective. Investigation into the error topology revealed the existence of hard-to-predict regions at the boundary between the elastic and plastic stages.

An instrumental breakthrough was the integration of an epistemic Uncertainty Quantification mechanism into the neural network architecture via MC Dropout layers. Analysis proved a strict correlation between regions of high model prediction variance and local sparsity of training points. This served as a trigger for a paradigm shift towards Active Learning. Rather than passive population, the surrogate model autonomously flagged parametric zones with the highest uncertainty, triggering the generation of new FEM computations precisely in these locations. Bridging these "information gaps" between existing clusters broke the convergence crisis, consistently reducing displacement errors to an acceptable level for engineering practice of 1.5 mm across a total database volume exceeding 50,000 validated samples, while the median error dropped to 0.672 mm.

PROPOSED NEURAL NETWORK ARCHITECTURE

Instead of directly predicting the three-dimensional displacement field $\mathbf{U}\ (x, y, z)$, this study proposes a novel approach based on PINNs utilizing kinematic decomposition. The overall displacement field is partitioned into the displacement vector of the idealized beam axis (macro-kinematics) and the vector of its local warping:

$$\mathbf{U}_{\text{total}}(x,y,z) = \\ = \mathbf{U}_{\text{spine}}(x) + \mathbf{R}(x)\cdot\mathbf{U}_{\text{warping}}(y,z)$$

where $\mathbf{U}_{\text{total}}$ is the total spatial displacement vector of an arbitrary cross-section point;
$\mathbf{U}_{\text{spine}}$ is the displacement vector of the idealized beam axis (macro-kinematics);
$\mathbf{R}$ is the spatial section rotation matrix;
$\mathbf{U}_{\text{warping}}$ is the vector of local micro-warping in the section plane.

To overcome parameter competition and achieve unprecedented computational speed, a four-stage cascade architecture consisting of sequential specialized modules was developed [5, 9]. The first stage utilizes a multi-label neural network acting as a Pre-Filter Gate, which identifies non-physical samples and cases of unstable buckling, instantaneously rejecting such configurations prior to the execution of the main macro-model. This solution, coupled with physical checks based on the von Mises criterion, reduces the number of missed critical states to practically zero, guaranteeing the highest reliability for the optimizer. The second stage is a plasticity classifier built on the Mixture-of-Experts principle, which determines the probability of assigning the problem to the elastic or plastic stage, functioning as a router for subsequent system components. The third module is the core Skeleton PINN network, tasked with approximating global macro-kinematics, including deflections along all spatial axes and twist angles along the idealized one-dimensional axis [7]. In the final stage, the Flesh PINN network utilizes these predicted macro-parameters as inputs to accurately reconstruct three-dimensional micro-stresses and warping directly within the beam cross-section [13]. To stabilize the training process of the entire system, logarithmic scaling of the loss function and dynamic weight balancing were applied. The general scheme of the developed cascade is illustrated in Fig. 3.

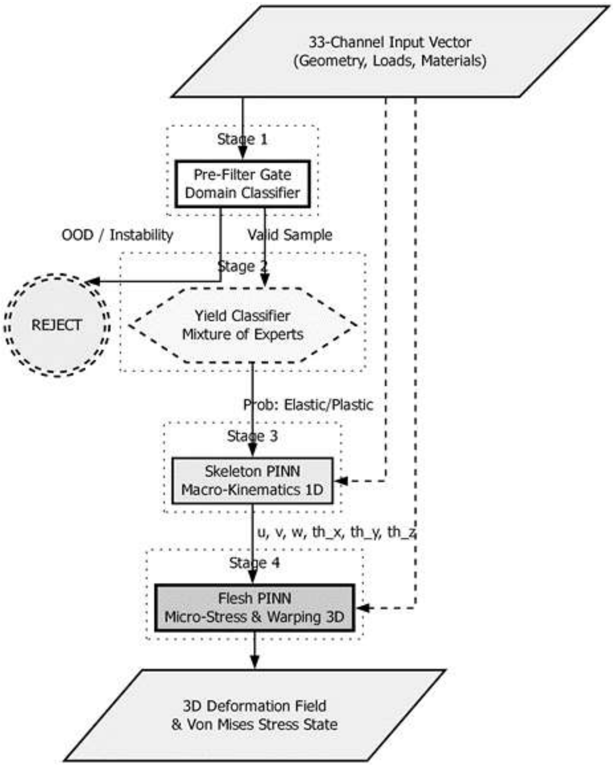

Fig. 3. Architectural diagram of the Four-Stage Cascade Physics-Informed Neural Network (PINN)

Рис. 3. Діаграма архітектури чотирьохкаскадної фізично-інформованої нейромережі (PINN)

UNCERTAINTY QUANTIFICATION

A crucial requirement for surrogates in structural engineering is predictability. The model implements an internal mechanism for estimating the accuracy of its predictions (Uncertainty Quantification) based on the use of MC Dropout layers during inference, coupled with KDTree Sparsity Distance algorithms.

This allows the network to generate spatial 3D Uncertainty Maps, where the variance of predictions directly indicates to the user the Out-of-Distribution regions where accuracy might be compromised (Fig. 4).

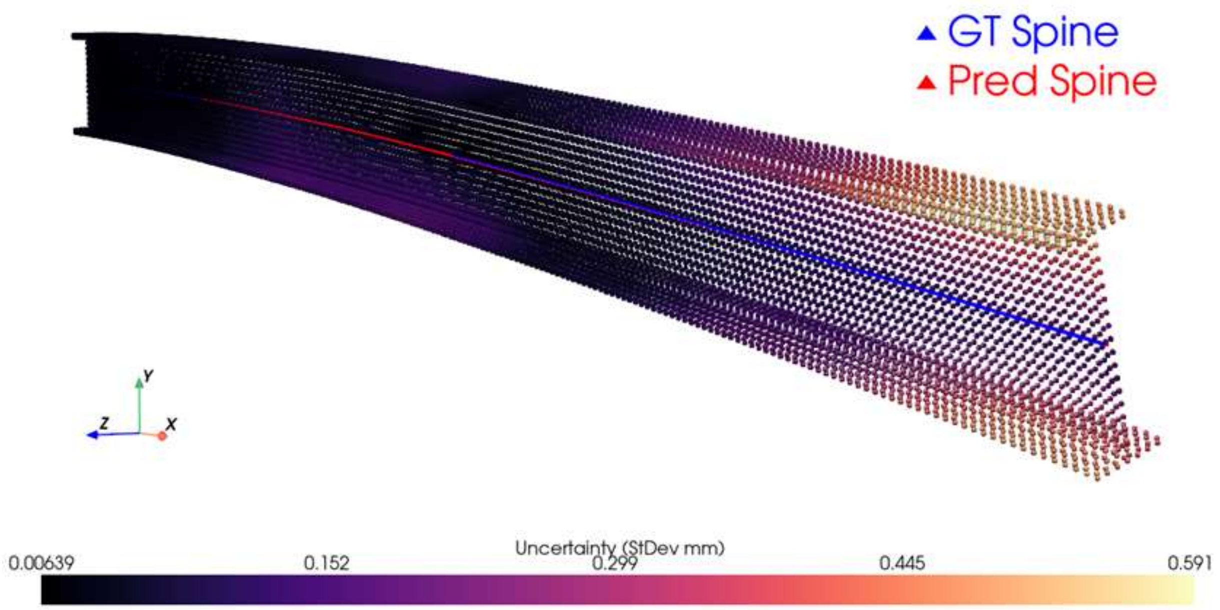

Fig. 4.3D Uncertainty Map
Рис. 4. 3D мапа невпевненості

EXPERIMENTS AND RESULTS

The rigorous experimental validation of the model was performed on completely isolated test sets, including extrapolative batches of a thousand samples representing complex spatial behavior, which confirmed that the surrogate's accuracy is commensurate with the results of traditional FEM computations. An analysis of the physical accuracy metrics (Table 1) and the distribution of median errors across test scenarios (Table 2) indicates high prediction stability. Upon completion of training, the Median Absolute Error (MedAE) of macro-deflection was 0.672 mm, while the 90th percentile value reached 3.453 mm. It is important to note that the mean absolute error even for the most complex edge-case domains stabilized at the level of 1.5 mm.

Table 1. Overall Physical Accuracy of the Surrogate Model (MAE Percentiles)
Табл. 1. Загальна фізична точність сурогатної моделі (персентилі середньої абсолютної похибки)

Physical Quantity	Median (P50)	90th Percentile (P90)	99th Percentile (P99)	Unit
Macro-deflection	0.672	3.453	11.630	mm
Von Mises Stress	1.985	5.281	13.404	MPa
Micro-warping	0.006	0.014	0.037	mm
Torsion	0.30	1.00	4.00	mrad

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Table 2. Distribution of Median Error (P50) across Test Scenarios
Табл. 2. Розподіл медіанної похибки (P50) за тестовими сценаріями

Spatial Behavior Scenario	Macro-deflection (mm)	Stress (MPa)	Warping (mm)	Torsion (mrad)
Pure Y- Bending	0.625	1.512	0.005	0.40
Lateral-Torsional Buckling	0.542	2.350	0.007	0.30
Compression with Flexural Buckling	0.655	1.333	0.002	0.10
Complex Spatial Chaos	0.820	2.236	0.006	0.30

Furthermore, regarding the internal micro-stresses, the median error is 1.99 MPa with the 90th percentile located at 5.28 MPa. Micro-warping is modeled with a median error of 0.006 mm, and for torsion, a virtually perfect match with the reference data was achieved, where the median error equals 0.30 mrad, and the 90th percentile is 1.00 mrad. The strategic application of the active learning mechanism enabled a six-fold reduction in the model's error in the most challenging zones characterized by extreme plasticity on the verge of instability (Fig. 5). The corresponding comparisons of deflection and stress curves, as well as cumulative error distribution plots, are presented in Figs. 6 and 7.

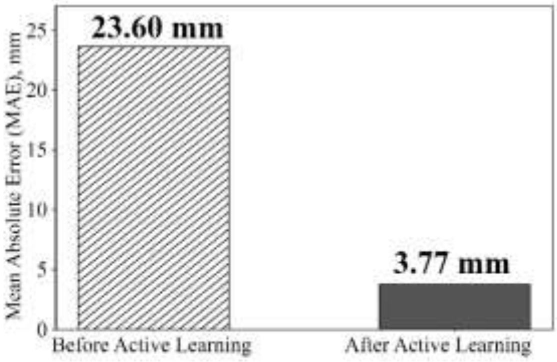
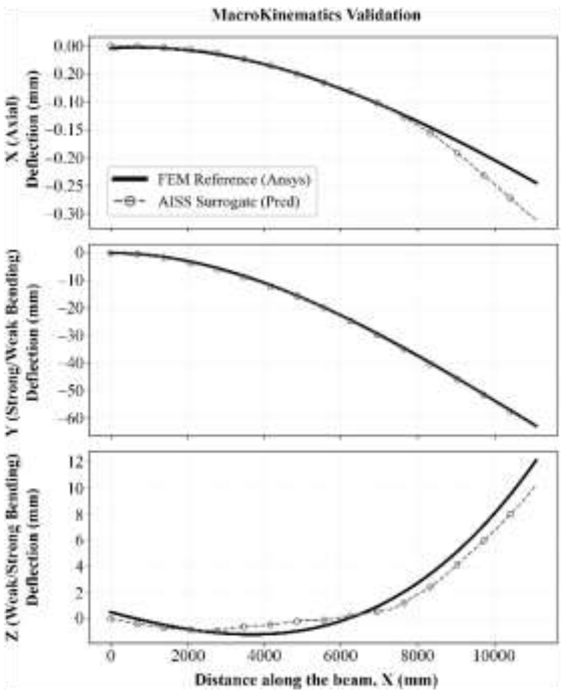


Fig. 5. Performance of the Active Learning algorithm: reduction of absolute error in marginal zones
Рис. 5. Ефективність алгоритму активного навчання: зниження абсолютної похибки в екстремальних зонах



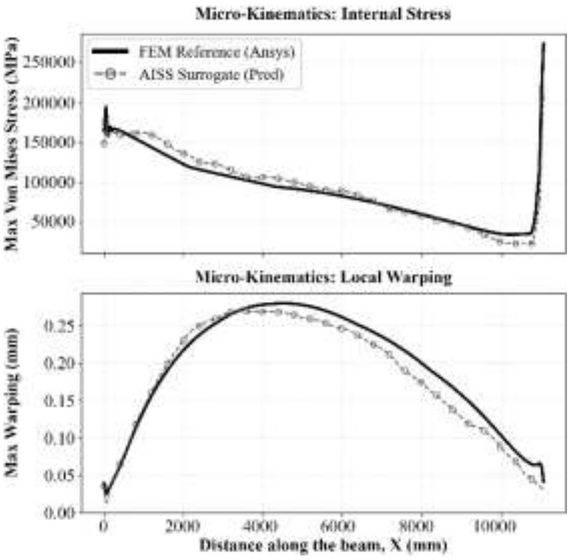


Fig. 6. Plasticity validation: AI vs. FEM
Рис. 6.Валідація пластичності: ШІ vs. МСЕ

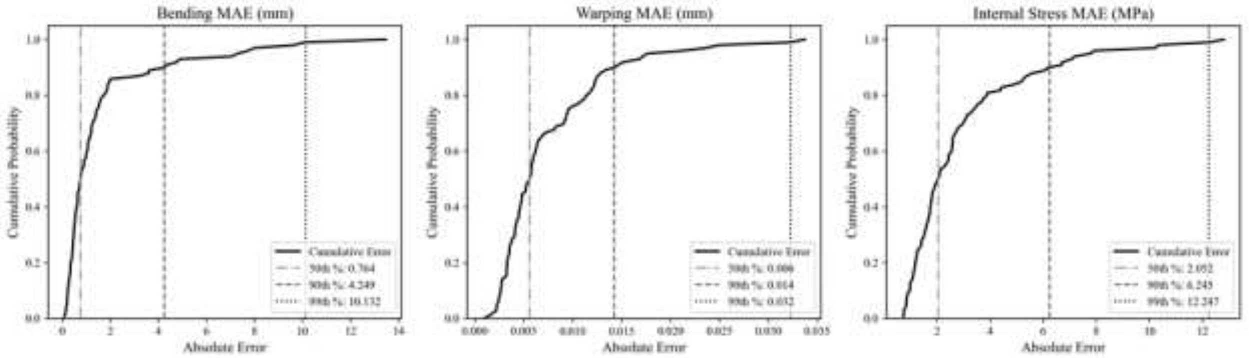


Fig. 7. Statistical error distribution
Рис. 7. Статистичний розподіл похибок

An Ablation Study of individual system components revealed a trade-off between computational speed and safety, which is realized through two available inference modes (Table 3). In the fast inference mode without epistemic variance estimation, the processing time for a single structural scheme in batch mode is only about 11.5 ms.

Table 3. Ablation Study – Comparison of Inference Modes
Табл. 3. Абляційне дослідження – порівняння режимів інференсу

Characteristic	Fast Mode	Safe Mode
Mechanism	Single Pass	15x passes of MC Dropout
Inference time per problem (GPU batch mode, batch size = 64)	~11.47 ms	~155.76 ms
False Positives	29.40%	31.90%
False Negatives	1.30%	0.90%

However, under these conditions, the rate of missed critical states (false-negative predictions) is 1.30%, and the level of excessive safety margin for safe configurations (false-positive predictions) is 29.40%. For tasks demanding elevated reliability, a Safe Mode is provided, employing fifteen passes of the MC Dropout algorithm alongside physical heuristics. The control of the upper confidence bound of the variance and von Mises stress verification minimize the number of missed critical states to an acceptable 0.90% for engineering applications, although the rate of falsepositive triggers increases to 31.90%. Such asymmetry indicates a strict conservative bias embedded in the model, prioritizing operational safety in marginal zones over the completeness of the search space. Despite the increase in average computation time to 156 ms in Safe Mode, the system is capable of pre-screening thousands of topological variations in the time equivalent to a single iteration of classical analysis in Ansys.

DISCUSSION: APPLICATION IN STRUCTURAL OPTIMIZATION

The achieved accuracy and speed metrics enable the efficient use of the surrogate model in subsequent iterative structural design cycles, such as when applying genetic algorithms or during the topology optimization of building frameworks [12]. The developed conceptual approach is highly scalable: provided the training dataset is appropriately expanded, the method can be easily adapted to other profiles, such as channels, T-sections, or pipes, as well as to atypical loading conditions. This development is considered a foundational component of a large-scale paradigm for creating an AI-based "structural toolkit". Future perspectives envision the development of a complete set of integrated structural model components, including neural network models for joints connecting columns and beams, floor slabs, and building roof structures [11, 14].

One of the most acute problems in applying surrogate models in automated generative design cycles of buildings is the presence of false-negative predictions capable of cementing an objectively unviable design as a global optimum. Through the implementation of hierarchical pre-screening within the Safe Mode, the developed neural network acts as a primary filter, instantly discarding over 99% of dangerous configurations, leaving exclusively potentially reliable variants in the search pool. The optimal macro-design, selected by the surrogate according to the target criteria of mass minimization of the structure, is forwarded for final rigorous verification via the finite element method. If this verification reveals a local exhaustion of load-bearing capacity in an individual structural element—indicating a scenario falling within the residual 0.9% statistical error of the model—the optimization system does not reject the found topology entirely. Instead, a local reinforcement algorithm (Smart Local Sizing) is initiated, which automatically increases the cross-section of the overstressed element [15]. The updated framework undergoes rapid re-validation by the surrogate model to assess the overall force redistribution and is subsequently returned to FEM analysis. Such a hybrid approach completely negates the impact of the residual AI error [6], preserving the high rank of the discovered design in the optimizer and guaranteeing absolute operational reliability of the final solution without an exponential increase in computational costs.

CONCLUSIONS AND PERSPECTIVES FOR FURTHER RESEARCH

The conducted research proves the capability of cascade PINN architectures to act as surrogate solvers in high-dimensional problems of nonlinear structural mechanics. The use of the kinematic decomposition method neutralized parameter competition by isolating the computation of global macro-kinematics from local micro-warping. It was established that a key factor in achieving engineering accuracy is the shift from static datasets to active learning algorithms guided by the model's internal uncertainty metrics.

The analysis of residual errors outlines the directions for further architectural development. The idea of stratifying the cascade by introducing a lightweight predictive module (prior-attention layer) possesses significant potential. This node would perform an initial approximation of the deformed axis on a discrete set of 10-15 control points, forming a spatial prior framework for the main continuous Skeleton PINN network, which would radically narrow the shape function search space.

Within the scope of the study, the problem of handling bifurcation phenomena was successfully resolved [10]. By delegating the recognition of buckling states to a specialized probabilistic classifier (Pre-Filter) in combination with von Mises stress calculation prior to main inference, it became possible to completely isolate singular anomalies. This allows the developed system to be transformed into a reliable and fail-safe computational core for parametric optimization and generative building design.

ETHICAL DECLARATIONS

The authors have no relevant financial or non-financial interests to report.

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КАСКАДНА ФІЗИКО-ІНФОРМОВАНА НЕЙРОМЕРЕЖЕВА СУРОГАТНА МОДЕЛЬ ДЛЯ БАГАТОВИМІРНОЇ СИМУЛЯЦІЇ СТАЛЕВИХ БАЛОК В УМОВАХ ПРУЖНО-ПЛАСТИЧНОГО ДЕФОРМУВАННЯ

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Анотація. У сучасній будівельній механіці використання багаторазових оптимізаційних циклів для розрахункових схем просторових конструкцій вимагає значних обчислювальних ресурсів. Традиційний розрахунок методом скінченних елементів (МСЕ) забезпечує високу точність, проте є занадто повільним для ітеративної оптимізації, тоді як швидкі аналітичні розв'язки часто не володіють необхідною точністю, особливо за межами пружної роботи матеріалу. У цій роботі запропоновано сурогатну нейромережеву модель на основі фізико-інформованих нейронних мереж (PINN) для миттєвого передбачення деформацій та напружень у сталевих балках двотаврового перерізу. Модель враховує 33-вимірний параметричний простір, що включає геометрію, фізичні властивості матеріалів, 6-DOF навантаження на кінцях та розподілені навантаження. В основі лежить метод кінематичної декомпозиції та чотириетапна каскадна архітектура (Pre-Filter, Yield Classifier, Skeleton PINN та Flesh PINN). Завдяки використанню послідовності Халтона та механізму Active Learning для генерації бази даних (>50 000 зразків) з фільтрацією екстремумів за критерієм відносного прогину $L/50$, модель демонструє високу інженерну точність: медіанна абсолютна похибка (MedAE) прогину становить 0,672 мм, при цьому максимальна похибка для переважної більшості складних нелінійних задач (80–90% вибірки) не перевищує 1,5 мм. Напруження передбачаються з медіанною похибкою 1,99 МПа. Використання механізмів оцінки невпевненості (Uncertainty Quantification) у режимі «Safe Mode» у комбінації з фізичними евристиками (контроль напружень за Мізесом) дозволяє мінімізувати частку нерозпізнаних критичних станів (False Negatives) до 0,9% забезпечуючи строго консервативну поведінку моделі при збереженні високої швидкості інференсу (на контрольній системі час обчислення склав ~156 мс), що на порядки перевершує швидкість традиційного МСЕ. Крім того, розроблений підхід дозволяє ефективно інтегрувати сурогатну модель у багаторазові цикли генеративного проєктування та топологічної оптимізації будівельних каркасів

Ключові слова. сурогатне моделювання; будівельна механіка; метод скінченних елементів; Physics-Informed Neural Networks (PINN); Active Learning.

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