Neural surrogate-driven modelling, optimisation, and generation of engineering designs: A concise review

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Abstract. Synergies between neural networks and traditional surrogate modelling techniques have emerged as the forefront of data-driven engineering. Neural network-based surrogate models, trained on carefully selected experimental data or high-fidelity simulations, can predict behaviours of complex systems with remarkable speed and accuracy. This review examines the current state and recent developments in neural surrogate technologies, highlighting their expanding roles in engineering design optimisation and generation. It also covers various feature engineering methods for representing 3D geometries, the principles of neural surrogate modelling, and the potential of emerging AI-driven design tools. While feature engineering remains a challenge, especially in parameterising complex designs for machine learning, recent advancements in code/language-based representations offer promising solutions for digitalising various design scenarios. Moreover, the emergence of AI-driven design tools, including text-to-CAD models powered by large language models, enables engineers to rapidly generate and evaluate innovative design concepts. Neural surrogate modelling has the potential to transform engineering workflows. Continued research into geometric feature engineering, along with the integration of AI-driven design tools, will speed up the use of neural surrogate models in engineering designs.

Introduction

Engineering design is the systematic process of conceiving, developing, and optimising products or services to fulfil specific needs and requirements [1]. Traditionally, this process relies on physical prototyping, repetitive simulations and human intuition, often leading to a time-consuming and potentially suboptimal outcomes. Advancements in machine learning (ML) technologies, particularly neural networks, are addressing longstanding challenges in this field by automating repetitive tasks [2], optimising designs for specific goals [3,4], and generating entirely new design concepts [5].

ML refers to the automatic mapping of underlying function(s) between input features and the desired output by optimising model parameters using observed data. ML models leverages probability theory to identify (learn) and approximate (fit) data distributions [6], enabling them to make predictions without explicit programming [7]. Feature engineering is a critical process in ML where raw data is transformed into meaningful features (inputs) to improve the performance and accuracy of the model [8]. It encompasses feature abstraction, which extracts meaningful patterns from complex raw data, and parameterisation, the process of defining and adjusting parameters of a model for optimal performance. In engineering contexts, feature engineering focuses on the abstraction and parametrisation of geometric information and performance-related attributes from relevant systems, processes or machines.

Digital twins are virtual replicas of the real world, serving as a key driver of the Fourth Industrial Revolution. They use real-time data to simulate physical systems, identifying issues and enhancing real-world performance [9]. For instance, Google Maps serves as the digital twin of the planet's surface, enabling navigation and virtual exploration [10]. Engineering digital twins typically leverage existing computer-aided design (CAD), computer-aided engineering (CAE) and computer-aided manufacturing (CAM) tools, which are tailored to various stages of the product lifecycle. Surrogate modelling, which creates simplified mathematical approximations of complex systems, has emerged as a vital component of digital twins [11]. The superior speed and data efficiency of neural networks make neural surrogate modelling ideal for industrial design applications [12,13]. Its computational efficiency enables rapid exploration of high-dimensional design spaces, a significant advantage over traditional simulation-heavy design approaches [14].

Emerging AI-driven design tools are further transforming the engineering design cycle [2]. Cloud-based ML platforms are streamlining the development of neural surrogates for engineers [15,16]. Generative design software autonomously creates design options, guided by performance requirements and manufacturing constraints [17]. Additionally, text-to-CAD (TTC) models can convert natural language descriptions into CAD-ready geometries [18,19]. The synergy of these technologies enables rapid generation, evaluation and optimisation of engineering designs.

This concise review aims to elucidate the frontier of neural surrogate technologies and their expanding applications in engineering design optimisation and generation. It explores different geometric feature engineering techniques, advancements in surrogate modelling for industrial design tasks, their integration with optimisation algorithms, and finally, capabilities of emerging AI-driven design tools. By examining the latest research developments in neural surrogate-driven engineering design, this paper offers insights into the future of this exciting field.

Geometric Feature Engineering

Geometric feature engineering involves the extraction, manipulation, and encoding of geometric properties into formats compatible with ML algorithms [8]. However, the lack of standardised, broadly applicable geometric feature engineering techniques has hindered the widespread adoption of ML in engineering.

Both numerical and categorical scalar data can be directly fed into scalar-based machine learning methods like support vector machines without extensive feature engineering [7]. In contrast, 2D information, typically in the form of pixel images, is typically processed through machine vision techniques such as convolutional neural networks (CNNs) [7]. The digital representation of 3D data is more complex, with diverse methods employed without a standard approach. A common technique involves projecting 3D objects into 2D profiles, enabling the application of image-based machine learning techniques [3,14]. While 3D projections of CAD models were utilised in several deep learning studies [20,21], this image-based representation of 3D shapes is often restricted to simple objects without internal features.

Other computational techniques frequently used for representing 3D geometry include voxel-, point cloud-, mesh-based, and implicit representations. Fig. 1 illustrates these four 3D representation techniques' depictions of the Stanford Bunny. Point clouds (Fig. 1(a)) are collections of points in 3D space, defined by their spatial positions (x, y, z) and sometimes other attributes (like colour) [16]. Voxel grids (Fig. 1(b)), on the other hand, resemble 3D versions of pixels and can be considered as quantised and fixed-sized point clouds [22]. As shown in Fig. 1(c), polygon meshes connect vertices with polygonal faces to form surfaces, often with additional 2D information mapped onto the triangular surfaces of the polygons [23,24]. In contrast to the explicit representations that capture geometric information in discretised formats, implicit representations use continuous, infinite-resolution functions (e.g., signed distance functions) to define a volume's occupancy field [3,5], as illustrated in Fig. 1(d). The recent use of neural networks to learn compact latent representations of implicit functions has made implicit neural representations more memory-efficient and better suited for numerical optimisation [25]. Despite their prevalent use, those position-based representations are incompatible with modern CAD software that models engineering components using sequential and parametric commands [5,26].

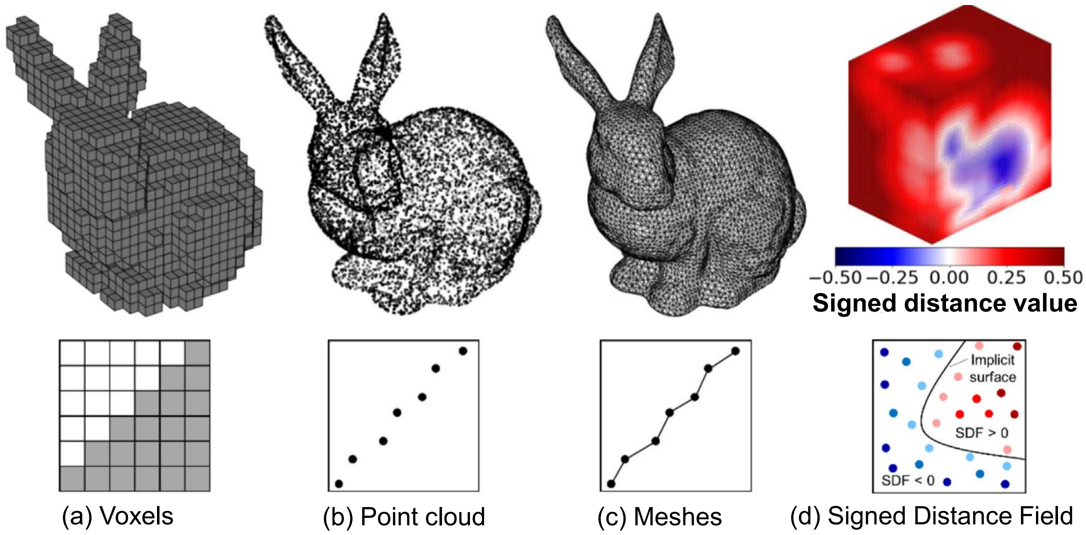
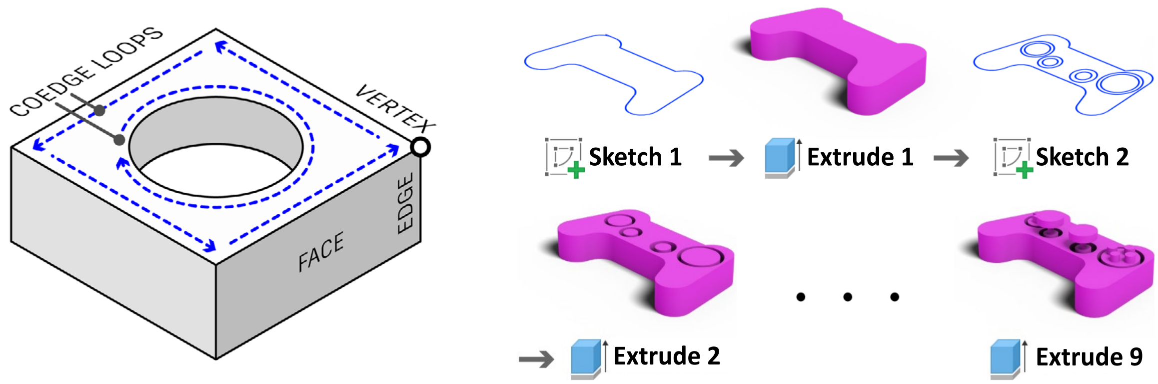


Fig. 1. Geometric representations of the Stanford bunny through explicit forms such as voxels (a), point cloud (b) and meshes (c), and implicit representations like signed distance fields (d) [25].

Given the rising prominence of large language models (LLMs) like ChatGPT, recent research in geometric feature engineering is pivoting towards code/language-based representations of 3D geometries [5]. These methods mainly encompass the boundary representation (BREP) techniques and CAD sequence-based representations, as shown in Fig. 2(a) and 2(b), respectively. The BREP format defines the boundary between the interior and exterior of a solid's volume using a collection of connected surface segments (Fig. 2(a)), complemented by topological information that explains their adjacency relationships [27]. In contrast, most CAD programmes use command (construction) sequences to create models, as shown in Fig. 2(b). This parametric representation allows one to model complex geometries using several parameters, without manually building it up from scratch [26]. The BREP serves as an abstraction of the CAD command sequences [26]. While viewable in most CAD software, BREP files lack the parametric history needed for direct modification using those tools. Additionally, the vocabulary formed by CAD command sequences is analogous to natural language. This similarity has encouraged the exploration of Autoencoder (AE)-based Transformer networks to produce command sequences of novel 3D CAD designs, which can be directly edited by users [26]. Furthermore, fine-tuned LLMs can generate construction sequences of CAD models based on user prompt inputs. These sequences can then be imported into existing CAD software to construct the final 3D model [19].

AEs are neural-network architectures designed for unsupervised learning tasks, particularly focusing on dimensionality reduction and feature extraction [7]. During the encoding process, AEs automatically identify a user-specified number of features from the input data, transforming them into latent encodings. These encodings are then used to reconstruct the output information in the decoder stage [28]. In engineering design, AEs can function as geometric feature detectors, providing more insightful or nuanced ways to describe geometries than human-designed methods [7,29]. For example, a latent parameter extracted from an input 3D surface mesh might represent a combination of lean and sweep of a compressor blade in turbomachinery [28].



(a) Modified from Lambourne et al. [27] (b) Adapted from Willis et al. [30]

Fig. 2. Code/text-based representation of 3D shapes – Boundary representation with its face-adjacency graph (a); And CAD command (construction) sequence (b).

Surrogate Modelling

Surrogate modelling is a computational strategy that utilises intelligently sampled data to approximate complex mathematical models in unobserved regions of the design space [11]. Unlike purely data-driven methods, surrogate-based design optimisation can leverage data generated from simulations, thus overcoming the data scarcity issue common in engineering design. These models solely rely on the input-output behaviour of the true function, without consideration for its internal workings [1]. Modern design of experiment (DoE) methods, such as the Latin hypercube sampling, were utilised to ensure efficient data collection and maximised sampling uniformity across the design space [11,31].

Classic surrogate modelling techniques such as polynomial response surface model, Kriging, and radial basis functions incorporate statistical learning principles, but they do not engage in "learning" as comprehensively as modern ML algorithms [11]. Conversely, ML-based surrogates, particularly neural networks, are less confined by predefined mathematical structures and excel at dimensionality reductions for very high-dimensional and non-linear problems [12]. Multi-layer perceptron (MLP), a class of feed-forward neural networks, is especially suitable for surrogate modelling of complex non-linear problems in engineering design [12]. These networks excel at predicting and optimising both scalar performance metrics and 2D/3D physical fields [12,14]. Owing to their rapid evaluation speed, neural surrogates can significantly accelerate certain engineering design processes by eliminating the need for the repetitive evaluation of time-consuming CFD or FEA codes [3,13].

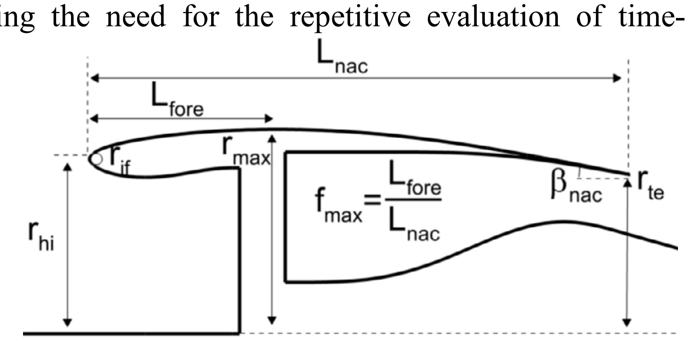


Fig. 3. Design variables used in the parametrisation of an aeroengine nacelle [32].

Neural surrogate models have become instrumental in predicting the performance of parameterised engineering designs [13]. Parametric design variables, such as those defined for the aeroengine nacelle of a civilian airplane (Fig. 3), were commonly used as inputs for the neural networks that predict performance metrics [32,33]. Tejero et al. modelled the nacelle drag characteristics across the design space, and under different operating conditions, using MLP networks [32]. Similar MLP networks were also employed to estimate the coefficients of lift and drag, pitching moment, and the lift-to-drag ratio based on the angle of attack and flap configurations for experimental aeroplane designs [33].

Beyond parametric design inputs and outputs, surrogate models are increasingly embracing image-based representations [14,34]. Fig. 4 depicts an image-to-image surrogate model employing AEs [3], which maps input images to corresponding output images [28]. Attar et al. [14] and Zhou et al. [34] used Res-SE-U-Net based image-to-image models to predict blank's thinning fields (as 2D image) from die geometry and blank shape images. Comparative analyses indicate that image-based neural surrogate models outperform their scalar-based counterparts in prediction accuracy, data efficiency, informativeness and generalisability [4,34,35].

In addition to images, neural surrogates can also process 3D input and output data [28,36]. For example, Pongetti et al. deployed a multi-level neural surrogate model to predict various quantities of interest, such as the static pressure field on turbomachinery compressor blades based on their 3D surface mesh input [28]. Moreover, Petrik et al. developed neural surrogate models for optimising open die forging processes [36]. These models accept the input of a 3D voxel mesh representing the pre-stroke geometry of the workpiece, along with a forging vector that defines the forging path. They output predictions of the recrystallisation and shape deformation of the corresponding workpiece in 3D space, both represented as voxel meshes. Results suggest that this system can accurately mimic simulations throughout the entire interpolation space [36].

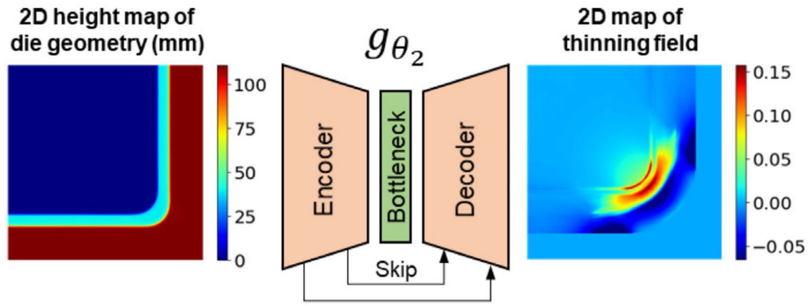


Fig. 4. Image-to-image surrogate modelling driven by an autoencoder [3].

Neural Surrogate-Driven Design Optimisation

Industrial and scientific endeavours are fraught with design problems that require the development of novel systems or processes for improved performance and efficiency [37]. Traditional design optimisation methods adopt a "top-down" approach where designers iteratively adjust design variables to achieve pre-defined performance metrics [13], often relying on trial-and-error or empirical strategies [4]. Given that modern engineering is primarily driven by expensive computer simulations [38], this process typically involves a non-exhaustive exploration of the design space, frequently resulting in suboptimal design outcomes [13]. In comparison, neural surrogate-assisted design optimisation incurs significantly lower computational costs, allowing near-instant evaluations of designs [4,38]. The fast surrogate modelling enables the optimisation algorithm to iteratively search for the optimal point(s) within the design space starting from an initial configuration [1]. As the outcomes of these optimisation processes are unforeseen, this constitutes a "bottom-up" approach [13]. Moreover, for optimisation problems, neural surrogate modelling helps imposing various boundary conditions, such as manufacturing and geometric constraints, by directly modelling them within the surrogate [3,4]. Ultimately, highly accurate and generalisable neural surrogates pave the way to be integrated within full-function digital twins, enabling real-time, multi-objective design optimisation [4].

Surrogate-driven design optimisation has been prevalent in aerodynamic design, encompassing aeroplane components [32,33], turbomachinery [28], flight envelopes [39], etc. Norgaard et al. determined the optimal flap settings and flap schedule for a research airplane by employing neural networks to predict performance metrics [33]. Leveraging predictions of quantities of interest from 3D-to-3D neural surrogate models, Pongetti et al. iteratively refined the optimal geometry of turbine compressor blades with an evolutionary algorithm to solve the targeted optimisation problem [28]. Additionally, the optimal landing trajectory for a spacecraft was determined using gradient descent optimisation based on aerodynamic predictions from neural surrogates [39].

Neural surrogate modelling also finds extensive application in the metal forming sector, particularly for optimising tooling design and process parameters vital to the cost and quality. Due to the intricate nature of these manufacturing processes, slight adjustments can result in significant changes in manufacturability metrics, rendering the traditional design process slow and error-prone [4]. Sheet metal forming processes rely heavily on optimal blank shapes, but scalar-based surrogate models, limited by accuracy, robustness, generalisability and the data inefficiency, struggled in the modelling and optimising blank shapes [4,34]. Attar et al. leveraged non-parametric neural surrogates capable of handling intricate morphing geometries, and gradient-based algorithms, to optimise geometries of hot stamping dies and blank shapes for corners and bulkheads. These geometric adjustments driven by manufacturability predictions resulted in notable enhancements in component quality [3]. Furthermore, CrystalMind's surrogate models for optimising open-die forging processes are coupled with a dual annealing-based optimisation algorithm, which iteratively adjusts the forging vector to achieve deformation and recrystallisation patterns that closely match target outcomes. The rapid feedback of these neural surrogates enables the optimisation process to finish much faster than with FEA simulations [36].

Emerging AI-driven Design Tools

Digital transformation in engineering industries has primarily focused on surrogate modelling of engineering products and processes, frequently leveraging raw CAD and CAE data [16]. This approach has enabled faster design iterations and higher product quality [16], effectively addressing the slowness of traditional CAD and CAE tools [15]. Web-based platforms such as NeuralConcept and Monolith AI offer streamlined software solutions to engineers that facilitate surrogate-driven design evaluation and optimisation [15,16]. These enterprise AI infrastructures integrate the cutting-edge deep learning algorithms with a user-friendly interface into a modular platform, enabling users to rapidly create and scale up various types of surrogate models using cloud computing resources [15]. By minimising coding requirements and providing comprehensive guidance on ML, these end-to-end platforms make powerful machine learning tools accessible to mainstream engineers [16]. Industrial applications of these AI platforms demonstrate significant saving in engineering time. For instance, a car manufacturer slashed the development period of a new vehicle from five years to just one after adopting this solution [15].

Additionally, tools for generative topology optimisation, also known as generative design, have been introduced in leading CAD programmes [17]. This technology automates the creation and iterative modification of a component's topology, based on user-defined performance requirements and manufacturing constraints [17]. Topology optimisation tools work by iteratively refining the geometry of a design until it converges to an optimal solution that satisfies all objectives and constraints. In comparison, generative topology optimisation produces multiple design choices that satisfy specified design requirements. More advanced versions even rank generated design options to facilitate user evaluation [17]. These tools are often integrated with CAE software for design evaluation, a process that neural surrogate modelling can greatly expedite. Some of them also incorporate CAM functionalities to impose design constraints [17].

Text-guided generative AI models that can produce 2D images, 3D geometries and sequences of programming languages, are quickly emerging in both academic and industrial sectors [18,40,41]. Text-to-image generators like the DALL-E series, Imagen and Midjourney, have been utilised to produce high-quality images of design concepts, especially in architecture [42]. Similarly, text-to-3D models generate various parameterised 3D geometries (point cloud [43], textured mesh [43], implicit neural radiance fields [44], etc.) from text input. These models are widely applicable in 3D content creation for gaming, virtual reality and industrial design [43]. TTC models, on the other hand, produce parametric command (construction) sequences that adhere to existing CAD file formats, making them directly importable into most CAD software [18,19,41]. As shown in Fig. 5(a), one TTC app facilitates parametric editing of CAD objects based on user's

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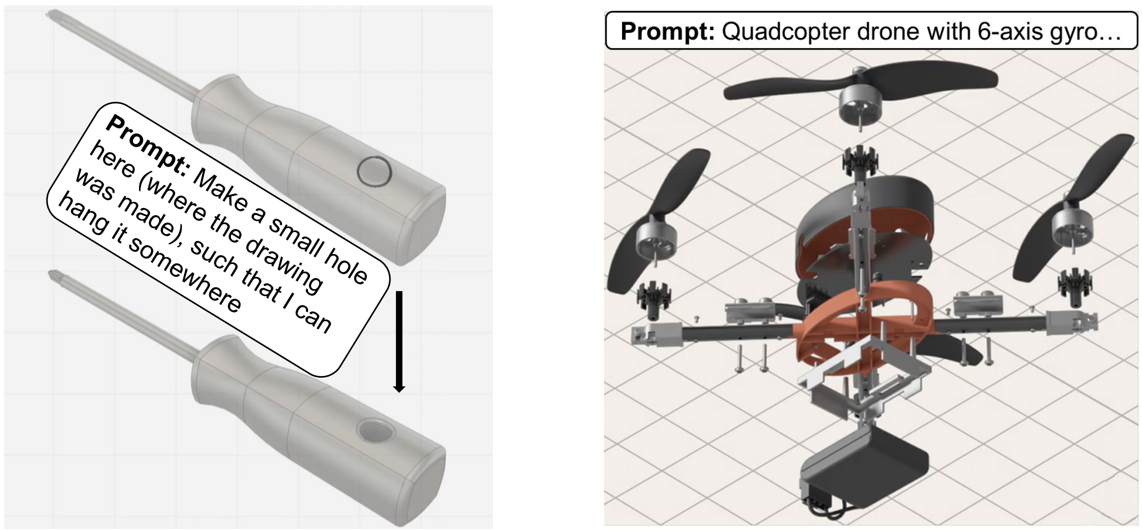
command prompts and drawing inputs [40], while another supports the generation of complex, fully-mated assemblies (Fig. 5(b)) [41]. Moreover, some TTC models offer "copilot" features like the autocompletion of CAD files [18]. These functionalities are derived from the models' deep understanding of both CAD file syntax and its correlation to 3D geometry. By training on open-source or proprietary datasets of engineering designs, these models learn to effectively leverage historical design information to synthesise new designs [19]. Certain platform even allows for fine-tuning of the pre-trained TTC models to users' specific database [19], further bolstering the benefit of this AI infrastructure. These text-to-design tools enable novice users to exploit insights from past design data and assist experienced designers to quickly visualise and explore innovative design concepts. In near future, the capabilities of TTC models are expected match the LLMs that power them. This will unlock extraordinary geometric inference capabilities, transforming the way designers interact with complex shapes. With the incorporation of neural surrogate modelling, these generative AI models can instantly assess created designs, thereby intelligently guiding the optimisation of complex design cases.



(a) CadifyAI [40] *(b) GetLeo.ai* [41]

Fig. 5. AI-powered generation and modification of CAD parts and assemblies: Text prompts and drawing inputs allow for real-time model modification (a); Complex, fully-mated assemblies of engineering designs are generated from scratch using simple text instructions (b).

As AI-powered design tools become more accessible, they are poised to transform numerous engineering practices. These tools are devised to augment the capabilities and efficiency of human designers, who remain the principal decision maker, instead of replacing them [45]. Looking ahead, future developments incline towards merging these technologies to create full-function digital twins that will intelligentise the design and manufacturing of engineering products.

Summary

This review represents a pioneering survey of how neural surrogate technologies can revolutionise reduced-order modelling, optimisation and generation of engineering designs. Despite challenges in geometric feature engineering for complex hardware designs, neural surrogate modelling stands out as a substantial advancement over traditional CAE methods. Neural surrogates empower the broader use of optimisation algorithms and enable the exploration of extensive design variations, potentially shortening design cycles and improving product performance. Furthermore, emerging AI-driven design tools and infrastructures are reshaping engineering practices, supporting engineers throughout the design process. Integration of neural surrogate modelling with these AI-driven tools brings the realisation of comprehensive digital twins, a cornerstone of Industry 4.0

initiatives, closer to reality. The creation of comprehensive and accurate digital twins necessitates powerful modelling methods, thus underscoring the critical need to advance neural surrogate technologies. Future research into ingenious geometric feature engineering techniques, and the strategic integration of novel AI-driven design tools, is imperative for facilitating the widespread adoption of neural surrogate modelling across various engineering domains.

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