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Intelligent Computation and Analysis of Mechanical Behaviour in Piezoelectric Metamaterials Based on Physics-Informed Neural Networks

Danyang Qiu*, Yaoxin Huang, Xinru Li, Ningping Zhan

Faculty of Mechanical Engineering and Mechanics, Ningbo University, Ningbo 315211, China

Corresponding author: Danyang Qiu, 236001543@nbu.edu.cn

Abstract: Piezoelectric metamaterials, serving as critical functional media in high-end equipment, face significant design challenges due to the mesh bottlenecks of traditional finite element methods and the interpretability shortcomings of purely data-driven models. Physical Information Neural Networks (PINNs) establish a robust scientific machine learning paradigm by embedding physical equations, offering an innovative solution to these predicaments. This paper systematically reviews recent advancements of PINNs in piezoelectric metamaterial analysis and design: drawing upon multiscale modelling theory, it elucidates PINNs' mesh-free advantages in handling high-dimensional parameters and their exceptional capability in solving small-sample inverse problems; subsequently, it explores their application paradigms in constructing high-fidelity forward surrogate models and accelerating efficient topology optimisation. Finally, this paper summarises key computational challenges in multi-physics coupling scenarios and outlines potential pathways towards achieving high-fidelity intelligent design, aiming to bridge the existing gap between theoretical modelling and engineering practice in piezoelectric metamaterials.

Keywords: Piezoelectric Metamaterials; Physical Information Neural Network; Multi-Scale Modeling; Multiphysics Coupling; Topology Optimization

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1.Introduction

Piezoelectric metamaterials achieve artificial customisation of electromechanical coupling effects by overcoming the physical limitations of natural materials through sophisticated topological design and periodic arrangement of microscopic unit cells [1]. This novel intelligent medium exhibits exceptional properties including all non-zero piezoelectric coefficients, broad bandgap tunability, and negative Poisson's ratio [2-4], holding significant engineering value in fields such as aerospace vibration suppression, self-powered MEMS sensing, and structural health monitoring [5]. As engineering demands evolve towards extreme and precision requirements, the design specifications for piezoelectric metamaterials have expanded from simple mechanical load-bearing to complex "force-electricity-heat" multi-field coupling and anisotropic customisation. This significantly increases the complexity of microstructure topology optimisation design.

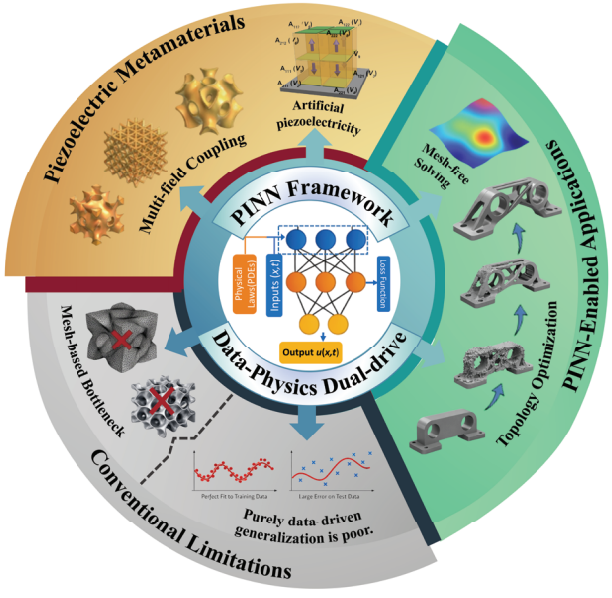
For a considerable period, mesh-based numerical methods such as the finite element method (FEM) and boundary element method (BEM) have been the mainstream tools for analysing piezoelectric structures. Whilst these methods demonstrate

maturity in conventional problems, they face significant challenges when handling piezoelectric metamaterials due to the high-dimensional parameter space and strong multi-field coupling calculations. On one hand, the piezoelectric effect involves strong bidirectional coupling between stress and electric fields. The disparity in magnitude between physical fields readily leads to deterioration in the condition number of the stiffness matrix, thereby compromising computational convergence. On the other hand, the introduction of intricate microstructures—such as triple-periodic minimal surfaces (TPMS) or fractal structures [6]—to pursue extreme performance renders high-fidelity meshing a computational bottleneck. Particularly in multiscale analysis and topology optimisation scenarios[7,8], computational load increases exponentially with degrees of freedom, rendering traditional numerical methods inadequate for real-time simulation and rapid iterative design requirements.

In recent years, deep learning techniques have offered novel avenues for alleviating the aforementioned computational bottlenecks[9]. Data-driven surrogate models have demonstrated application potential in accelerating structural response prediction and aiding additive manufacturing(AM) [10,11]. However, existing purely data-driven models, such as Convolutional Neural Networks (CNNs), typically lack physical interpretability and do not explicitly incorporate physical governing equations as constraints. This results in models being highly dependent on high-quality labelled data. In piezoelectric metamaterial research, acquiring high-fidelity ground truth datasets covering multi-field coupling and complex geometries is costly and challenging. Furthermore, the absence of embedded physical constraints means predictions from purely data-driven models cannot guarantee strict adherence to energy conservation or boundary conditions. Consequently, their generalisation performance beyond the training sample domain (out-of-distribution) is limited, hindering direct application in engineering design requiring high reliability.

To address these limitations, Raissi et al. proposed the Physical Information Neural Network (PINN), establishing a scientific machine learning (SciML) framework that integrates physical principles for solving complex partial differential equations (PDEs) [12]. By embedding the residuals of the partial differential equations governing the physical system as a regularisation term within the loss function, PINN achieves high-accuracy solutions for multi-physics problems without mesh generation and relying solely on sparse observational data. This dual ‘data-physics’ driven characteristic confers significant advantages in handling complex boundary conditions of piezoelectric metamaterials, multi-field coupled inverse problems, and parameter identification[13,14], and has been extensively validated for effectively resolving diverse engineering PDE problems[15]. In recent years, topology optimisation methods based on PINN have also seen progressive development and application[16]. This paper aims to provide a systematic review of the latest research advances in PINNs for analysing the mechanical behaviour of piezoelectric metamaterials, multi-physics coupling modelling, and topology-optimised design. The complete framework is illustrated in Fig. 1.

Figure1: Current status of computational studies on piezoelectric metamaterials within the PINN framework



To present the research trajectory of this emerging field with logical clarity, the subsequent sections of this paper are organised as follows: Section 2 elaborates on the physical modelling theory of piezoelectric metamaterials, establishing the necessity of introducing deep learning by analysing the multiscale computational bottlenecks of traditional methods; Section 3 systematically constructs the theoretical framework of PINNs, thoroughly comparing their advantages over finite element methods (FEM) and purely data-driven models; Section 4 focuses on core application strategies and cutting-edge developments of PINN in performance forward prediction and structural inverse design; Section 5 outlines future research directions for PINN.

2.Modelling the Mechanical Behaviour of Piezoelectric Metamaterials

The design and application of piezoelectric metamaterials hinge upon a profound understanding of their complex mechanical behaviour, with the core challenge lying in accurately describing the interaction between multi-physics coupling effects and multi-scale geometric features. This section aims to establish a systematic physical modelling theoretical framework spanning from microscopic mechanisms to macroscopic responses. Building upon the derivation of multi-field coupled governing equations using linear piezoelectric theory and continuum mechanics, alongside the establishment of physical conservation laws, this framework further elaborates on the representative volume element (RVE)-based equivalent medium theory and homogenisation methods. This addresses the unique periodic microstructural characteristics of metamaterials, thereby establishing a theoretical bridge mapping microscopic topological parameters to macroscopic effective material properties. Concurrently, addressing numerical bottlenecks arising from strong multi-physics coupling and complex geometries, this work thoroughly examines critical challenges such as ill-posed stiffness matrices and mesh distortion. This aims to establish a robust theoretical foundation for subsequent efficient analysis and topological optimisation.

2.1 Control Equations for Piezoelectric Dielectrics and Multi-Field Coupling Mechanisms

The macroscopic mechanical response of piezoelectric metamaterials is fundamentally governed by the bidirectional interaction between elastic and electric fields. This intrinsic electromechanical coupling effect manifests as the reciprocal processes of mechanical deformation inducing electrical polarisation (direct piezoelectric effect) and external electric fields exciting mechanical strain (reverse piezoelectric effect), endowing the material with exceptional performance in wave field manipulation and energy conversion. To quantitatively characterise this intricate dynamic physical process, a comprehensive mathematical model must be established within the framework of continuum mechanics and linear piezoelectric theory. Under the assumptions of small deformation and quasi-static electric fields, its physical behaviour is governed by the combined action of geometric equations, constitutive equations, and equilibrium equations. This yields a closed system of partial differential equations describing the mechanical behaviour of piezoelectric media[17].

Consider a piezoelectric continuum occupying spatial region $\Omega \subset \mathbb{R}^3$, whose boundary is

$$\partial\Omega = \Gamma_u \cup \Gamma_t = \Gamma_\phi \cup \Gamma_q \tag{1}$$

The displacement and potential are specified at Γ_u, Γ_ϕ, with natural boundary conditions applied at Γ_t, Γ_q.

Based upon the assumptions of a continuous medium, small deformations, and a quasi-static electric field, the geometric kinematics equations establish a consistent relationship between fundamental field variables and their gradient fields. Within the Cartesian coordinate system, for a given mechanical displacement vector u_i and electric potential scalar ϕ, the linear strain tensor ε_{ij} and electric field intensity vector E_i are respectively defined as:

$$\begin{cases} \varepsilon_{ij} = \dfrac{1}{2}(u_{ij} + u_{ji}) \\ E_i = -\phi_{,i} \end{cases} \tag{2}$$

The subscript comma denotes the partial derivative with respect to spatial coordinates. The symmetry of ε_{ij} reflects that rigid-body rotation does not induce strain, while the negative sign of E_i indicates that the electric field direction points from higher to lower potential.

The electromechanical coupling behaviour of piezoelectric materials is derived from the second-order expansion of the thermodynamic potential function. To facilitate the independent treatment of strain and electric field variations, $G(\boldsymbol{\varepsilon}, \mathbf{E})$ is selected as the fundamental thermodynamic potential, expressed as:

$$G(\mathring{\boldsymbol{a}},\mathbf{E})=\frac{1}{2}C_{ijkl}\varepsilon_{ij}\varepsilon_{kl}-e_{kij}E_k\varepsilon_{ij}-\frac{1}{2}\kappa_{ij}E_iE_j \tag{3}$$

The respective components correspond to elastic potential energy, electromechanical coupling energy, and dielectric energy. By taking partial derivatives of this potential function with respect to strain and electric field, the thermodynamic conjugates can be obtained:

$$\sigma_{ij}=\frac{\partial G}{\partial\varepsilon_{ij}},\quad D_i=-\frac{\partial G}{\partial E_i} \tag{4}$$

Constitutive equations serve as the link between force fields and electric fields, profoundly revealing the thermodynamic mechanisms of energy conversion within materials. Based on the above expression utilising Gibbs free energy or electric enthalpy density functions, linear equations in stress-charge form can precisely express the dependence of the stress tensor σ_{ij} and electric displacement vector D_i upon the independent variables of strain and electric field:

$$\begin{cases}\sigma_{ij}=C_{ijkl}\varepsilon_{kl}-e_{kij}E_k\\ D_i=e_{ikl}\varepsilon_{kl}+\kappa_{ik}E_k\end{cases} \tag{5}$$

This formulation simultaneously describes both the direct and inverse piezoelectric effects, ensuring the system satisfies energy conservation and the second law of thermodynamics.To systematically derive the control equations, an energy-based variational principle is introduced. For piezoelectric dynamics, the actual trajectory of the system should maximise the following functional:

$$\delta\int_{t_1}^{t_2}(T-\Pi)\mathrm{d}t=0 \tag{6}$$

Here, the system's kinetic energy is defined as:

$$T=\frac{1}{2}\int_\Omega\rho\dot{u}_i\dot{u}_i\mathrm{d}\Omega \tag{7}$$

Internal Energy (Electrical-Mechanical Coupling):

$$U=\int_\Omega G(\varepsilon_{ij},E_i)\mathrm{d}\Omega \tag{8}$$

External Forces and Electric Potential Energy:

$$W=\int_\Omega f_iu_i\mathrm{d}\Omega+\int_{\Gamma_t}\overline{t}_iu_i\mathrm{d}\Gamma+\int_{\Gamma_q}\overline{q}\phi\mathrm{d}\Gamma \tag{9}$$

Total potential energy:

$$\Pi=U-W \tag{10}$$

The internal energy is obtained by integrating the Gibbs free energy density over the entire domain, whilst the external work includes that performed by physical forces, surface forces, and surface charges. This constitutes a complete potential energy functional, providing a unified starting point for subsequent variational derivations.

By applying independent variational formulations to the displacement field and potential field respectively, and incorporating the variational relationship between strain and electric field, the variational representation of the energy functional can be expressed as an integral with respect to δu and $\delta\phi$. Applying Gauss's theorem to the spatial integral terms transfers the first-order derivatives from the variational function to the stress and electric displacement terms, thereby naturally introducing the corresponding boundary terms.

Displacement Variational:

$$\begin{aligned}\delta T&=\int_\Omega\rho\dot{u}_i\delta\dot{u}_i\mathrm{d}\Omega\\ \delta U&=\int_\Omega\left(\sigma_{ij}\delta\varepsilon_{ij}-D_i\delta E_i\right)\mathrm{d}\Omega\end{aligned} \tag{11}$$

Use:

$$\delta\varepsilon_{ij}=\frac{1}{2}(\delta u_{i,j}+\delta u_{j,i}),\quad \delta E_i=-\delta\phi_{,i} \tag{12}$$

Integration by parts in space (Gauss's theorem).

Stress term:

$$\int_\Omega\sigma_{ij}\delta u_{i,j}\mathrm{d}\Omega=-\int_\Omega\sigma_{ij,j}\delta u_i\mathrm{d}\Omega+\int_{\Gamma_t}\overline{t}_i\delta u_i\mathrm{d}\Gamma \tag{13}$$

Electrical displacement term:

$$\int_{\Omega} D_i \delta\phi_{,i} \mathrm{d}\Omega = -\int_{\Omega} D_{i,i} \delta\phi \mathrm{d}\Omega + \int_{\Gamma_q} \bar{q} \delta\phi \mathrm{d}\Gamma \tag{14}$$

Ultimately yielding the weak form of the piezoelectric dynamics problem:

$$\begin{aligned} &\int_{\Omega} \rho \ddot{u}_i \delta u_i \mathrm{d}\Omega + \int_{\Omega} \sigma_{ij} \delta\varepsilon_{ij} \mathrm{d}\Omega = \int_{\Omega} f_i \delta u_i \mathrm{d}\Omega + \int_{\Gamma_t} \bar{t}_i \delta u_i \mathrm{d}\Gamma \\ &\int_{\Omega} D_i \delta E_i \mathrm{d}\Omega = \int_{\Gamma_q} \bar{q} \delta\phi \mathrm{d}\Gamma \end{aligned} \tag{15}$$

The ultimate equilibrium state of the system is governed by physical conservation laws. For dynamical problems incorporating inertial effects, the mechanical field must satisfy the law of conservation of momentum (namely Newton's Second Law), whilst the electric field, under the assumption of an insulating medium, must satisfy the law of conservation of charge (namely Gauss's law from Maxwell's equations). Excluding physical forces and internal free charges, the governing equations may be expressed as:

$$\begin{aligned} &\sigma_{ij,j} + f_i = \rho \\ &\ddot{u}_i D_{i,i} = 0 \end{aligned} \tag{16}$$

Here, ρ denotes the material density, while $\ddot{u}_i$ represents the second derivative of displacement with respect to time. The aforementioned governing equations, coupled with the constitutive relationship and supplemented by corresponding mechanical boundary conditions (such as Dirichlet or Neumann boundaries) and electrical boundary conditions, constitute a complete boundary value problem for solving the wave dynamics and vibration characteristics of piezoelectric metamaterials.

In FEM, introduce interpolation:

$$\mathbf{u} \approx \mathbf{N}_u \mathbf{d}, \quad \phi \approx \mathbf{N}_\phi \varphi \tag{17}$$

Obtain a semi-discrete system:

$$\begin{bmatrix} \mathbf{M} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} \begin{bmatrix} \ddot{\mathbf{d}} \\ \ddot{\boldsymbol{\varphi}} \end{bmatrix} + \begin{bmatrix} \mathbf{K}_{uu} & \mathbf{K}_{u\phi} \\ \mathbf{K}_{\phi u} & -\mathbf{K}_{\phi\phi} \end{bmatrix} \begin{bmatrix} \mathbf{d} \\ \varphi \end{bmatrix} = \begin{bmatrix} \mathbf{f} \\ \mathbf{q} \end{bmatrix} \tag{18}$$

Where:

$$\mathbf{K}_{u\phi} = \int_{\Omega} \mathbf{B}^T e^T \mathbf{B}_\phi \mathrm{d}\Omega \tag{19}$$

2.2 Equivalent Medium Theory

he macroscopic properties of piezoelectric metamaterials are not solely determined by the intrinsic characteristics of the host material, but are primarily governed by the topological structure and periodic arrangement of their microscopic unit cells. This artificially engineered heterogeneity enables metamaterials to exhibit extraordinary electromechanical coupling properties at the macroscale that are difficult to achieve in natural materials[18-20]. To efficiently analyse extensive array structures at the engineering scale, the theory of equivalent media must be employed, approximating the microscopic non-uniform periodic lattice as a macroscopically homogeneous continuous medium [21]. The following sections introduce this approach through the definition of equivalent mechanical properties and the homogenisation principle.

Equivalent mechanical properties denote a set of averaged constitutive parameters capable of reproducing the physical response of microstructures at the macroscopic scale. For piezoelectric metamaterials, this process is commonly termed "homogenisation". Its theoretical foundation is established within a multiscale analysis framework and has been extensively applied to periodic composite materials[22,23].

The Representative Volume Element (RVE)-based volume averaging method combined with finite element analysis (RVE/FEM) is the most commonly employed homogenisation technique in engineering. It directly solves the unit cell response by applying periodic boundary conditions, offering advantages of intuitiveness and high accuracy[24]. The macroscopic mean stress $\bar{\sigma}ij$, mean strain $\bar{\varepsilon}ij$, mean electric displacement $\bar{D}_i$, and mean electric field $\bar{E}_i$ may be defined by integrating microscopic field quantities over the unit cell volume V:

$$\bar{\sigma}_{ij} = \frac{1}{V}\int_V \sigma_{ij} d\Omega \ , \ \ \bar{\varepsilon}_{ij} = \frac{1}{V}\int_V \varepsilon_{ij} d\Omega \tag{20}$$

By applying periodic boundary conditions (PBCs) at the cell boundaries and solving the boundary value problem, an

equivalent constitutive relationship describing the macroscopic behaviour can be obtained:

$$\begin{cases} \overline{\sigma}_{ij} = C_{ijkl}^{\text{eff}} \varepsilon_{kl} - e_{ijk}^{\text{eff}} E_k \\ \overline{D}_i = e_{ikl}^{\text{eff}} \varepsilon_{kl} + \kappa_{ik}^{\text{eff}} E_k \end{cases} \tag{21}$$

Among these, , and denote the equivalent elastic stiffness tensor, equivalent piezoelectric coupling tensor, and equivalent dielectric tensor respectively. These parameters constitute core metrics in metamaterial design—for instance, through microstructural engineering, one may achieve negative equivalent parameters unattainable in nature or significantly enhanced electromechanical coupling coefficients[25].

As computational complexity increases, so too does computational cost. To address this challenge, academia has developed multiple homogenisation strategies. Among these, Asymptotic Homogenisation (AH) offers the most rigorous mathematical foundation based on two-scale asymptotic expansion theory, capable of capturing higher-order correction terms. However, its derivation is cumbersome and struggles with extremely complex topologies[26,27]. In recent years, data-driven approaches have advanced rapidly, giving rise to new paradigms based on PINN and deep homogenisation frameworks. Such approaches achieve mesh-free, rapid prediction by learning mappings from microscopic structures to macroscopic equivalent properties, proving particularly suitable for complex topologies and inverse design [28, 29]. They provide efficient tools for optimising piezoelectric metamaterials and conducting multiphysics coupling analyses.

2.3 Multi-scale Structures and Computational Challenges

Piezoelectric metamaterials achieve customisation of macroscopic electromechanical properties through the periodic arrangement of microscopic topologies. While this cross-scale synergistic characteristic endows the material with extraordinary physical properties, it also poses significant challenges to conventional numerical computations. On the one hand, high-fidelity characterisation of microscopic geometric details leads to an exponential increase in computational degrees of freedom (DoFs) across the entire system. On the other hand, the inherent strong electromechanical coupling readily induces severe numerical ill-conditioning in the stiffness matrix. Consequently, overcoming computational scale explosion and convergence issues while maintaining physical fidelity has become the core bottleneck in current analysis and design.

2.3.1 Unusual physical properties arising from periodic structures

Periodic arrangements represent more than mere geometric repetitions of microscopic units. Wave dynamics analysis grounded in the Bloch-Floquet theorem demonstrates that such ordered structures can induce a series of singular dynamic responses. Firstly, these structures can form acoustic bandgaps, wherein elastic wave propagation is prohibited within specific frequency ranges. This property holds critical significance for broadband active vibration suppression in aerospace structures [30]. Secondly, through topological designs such as re-entrant or rotating rigid bodies, metamaterials exhibit negative Poisson's ratio effects, manifesting lateral expansion under tensile stress [31]. Research confirms that this counterintuitive kinematic behaviour significantly alters internal stress distributions, amplifying local effective strain on micro-piezoelectric elements by several orders of magnitud, thereby substantially enhancing macroscopic electromechanical conversion efficiency and energy harvesting power[32].

However, these complex microstructures are often accompanied by the phenomenon of local field enhancement, where the stress or electric field is highly concentrated at the interfaces of multiphase materials, forming "hotspots". Although previous studies have effectively alleviated the computational bottleneck and accuracy contradiction in piezoelectric fracture simulation by traditional finite elements through the adaptive isogeometric analysis framework based on PHT splines and other optimization methods[33], which improved the local mesh refinement technique (Fig2(a)), they are still fundamentally limited by the grid-based discretization solution path. When dealing with tasks such as real-time prediction, reverse design, or parameter inversion, they still face high costs of stiffness matrix reassembly and repetitive iterations. Such drastic gradient changes require numerical methods to have extremely high spatial resolution; otherwise, it is difficult to capture the true physical response.

2.3.2 Discretisation Bottlenecks in Complex Microstructure Topologies

To achieve high specific strength and multifunctional integrated performance, the unit cell configurations of modern piezoelectric metamaterials have evolved from simple truss structures to highly complex biomimetic continuous topologies. Typical examples include Triple-Period Minimal Surfaces (TPMS) and Hierarchical/Fractal Structures [34]. Such structures are often described by implicit level-set functions, featuring smooth, continuous surfaces and excellent topological properties. For these complex configurations, Wang et al. proposed a hybrid optimization framework integrating machine learning (ML) and evolutionary algorithms (EA) [35], demonstrating outstanding performance in the inverse optimization of biomimetic stress-strain curves for fractal metamaterials (Fig. 2(b)).

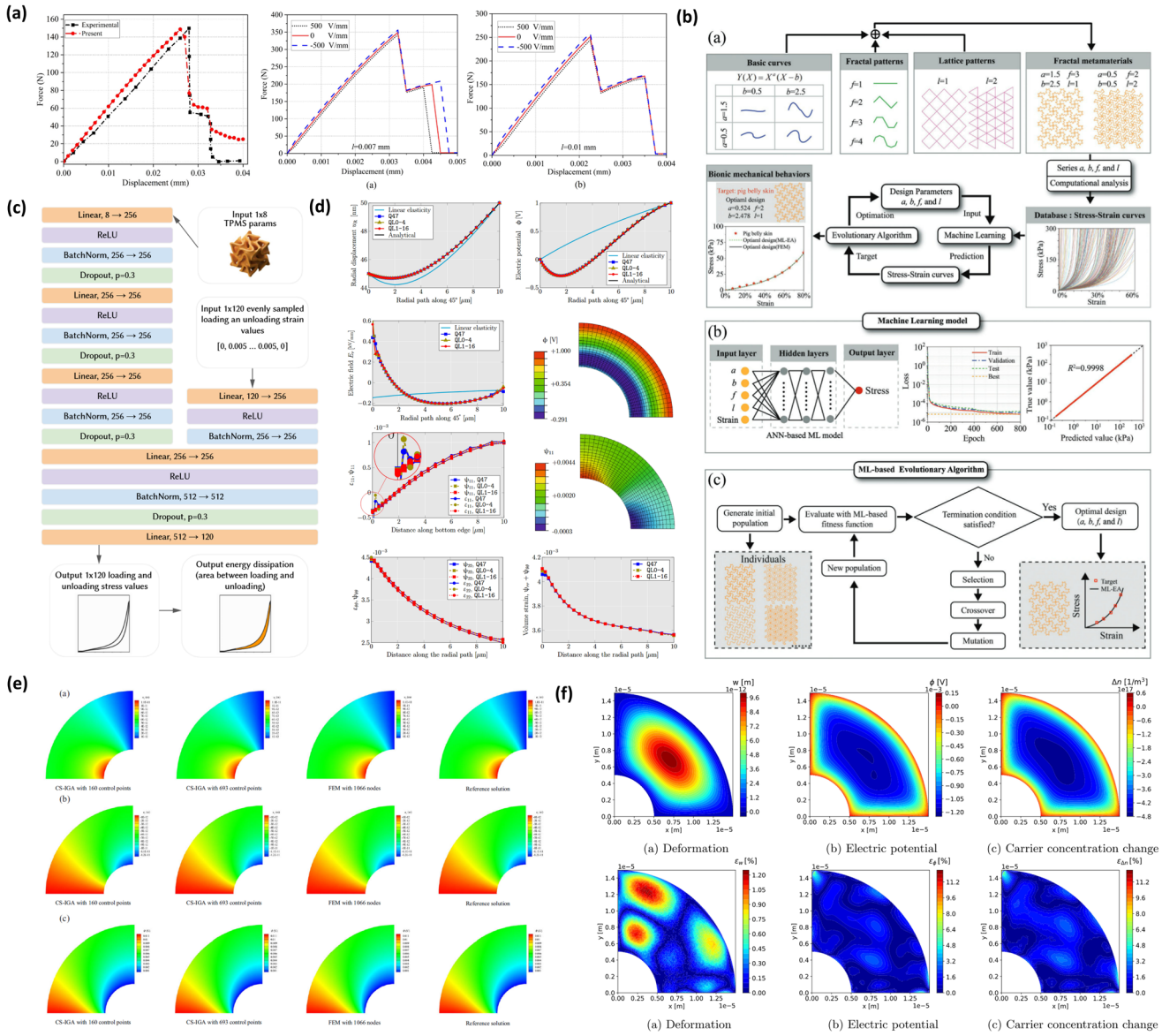
Despite the excellent mechanical potential of the aforementioned geometric design, its complex continuous topological features pose significant challenges for discrete numerical simulations. When employing traditional finite FEM, capturing surface curvature features with precision necessitates the generation of extremely dense unstructured tetrahedral meshes. Upon scaling up single cells to macroscopic arrays, mesh sizes grow exponentially into the tens of millions, frequently triggering out-of-memory errors [36] and resulting in extremely costly simulations and convergence issues (Fig. 2(c)). More critically, mesh distortion at complex surfaces readily induces singular Jacobian matrices and computational divergence, rendering high-fidelity topology optimization based on meshes impractical for engineering applications [37].

2.3.3 Multiphysics Strongly Coupled Stiffness Pathology

The analysis of mechanical behaviour in piezoelectric metamaterials confronts severe numerical stability challenges arising from strong multiphysics coupling. Unlike purely elastic problems involving single fields, piezoelectric analysis necessitates the coupled solution of momentum conservation equations and Maxwell's equations within a unified framework. However, these two physical fields exhibit a vast inherent disparity in energy and parameter scales: the elastic stiffness matrix typically reaches magnitudes of $10^{9} \sim 10^{11}$ Pa, whereas the dielectric constant is merely $10^{-9} \sim 10^{-11}$ F/m. This parameter difference spanning nearly 20 orders of magnitude directly results in the global system stiffness matrix, after discretisation, exhibiting extreme ill-conditioning, where the matrix condition number approaches infinity [38]. In traditional finite element method (FEM) analysis, such extremely poor condition numbers not only significantly amplify truncation errors in floating-point operations, causing conventional linear solvers to stagnate, but also induce severe volume locking or shear locking phenomena [39], necessitating supplementary optimization strategies (Fig. 2(d)).

Addressing this long-standing challenge, subsequent research has converged on a dual-track approach combining algorithmic reconstruction with data-driven methods. On one hand, discrete techniques based on smoothing or higher-order geometry have been shown to inherently suppress numerical locking caused by strong coupling at the mesh topology level (as illustrated in Fig. 2(e)), significantly reducing reliance on complex preprocessing techniques [40, 41]. On the other hand, with the emergence of PINNs, researchers began employing neural networks to solve piezoelectric partial differential equations. However, they also discovered that the aforementioned multiscale coefficient variations could lead to severe gradient singularities during optimization. To address this, recent work introduced a dimensionless normalization and adaptive loss weighting strategy [42], successfully achieving high-accuracy solutions for high-contrast multiphysics problems (Fig. 2(f)) without explicitly assembling massive stiffness matrices.

Figure 2: Addressing multiscale structures and numerical computation challenges. (a) An adaptive isogeometric analysis framework for PHT splines, alongside other optimisation methods, effectively mitigates computational bottlenecks and accuracy trade-offs in traditional finite element simulations of piezoelectric fracture by enhancing local mesh refinement techniques [33]. (b) A hybrid optimisation framework combining ML and EA demonstrates superior performance compared to traditional finite elements in inverse optimisation of biomimetic stress-strain curves for fractal metamaterials[35]. (c) A single multilayer perceptron model architecture within deep ensemble models resolves the extremely costly simulations and non-convergence issues associated with self-contact and large deformations [36]. (d) Experiment-driven Bayesian optimisation circumvents simulation bottlenecks for large deformations in complex structures, rigorously validated through physical experiments, analytical solution comparisons, or high-fidelity simulation data matching[39]. (e) Capability to resolve local accuracy loss issues caused by 'multiphysics strongly coupled ill-posed problems' through isogeometric analysis and smoothed finite elements[40]. (f) PINN resolves numerically ill-posed challenges arising from multi-field coupling, achieving high-precision solutions[42].



3. Overview and Comparative Analysis of the PINN Method

3.1 An Overview of the Fundamental Theory of PINN

With the introduction of the Physical-based Neural Network (PINN) by Raissi, Karniadakis et al.[12,14], a mesh-free computational framework integrating physical mechanisms was established by explicitly embedding physical governing equations into the deep learning optimization process (Fig. 3(c)). Unlike traditional purely data-driven approaches, PINNs directly map spatial and temporal coordinates to physical field variables. They utilise automatic differentiation (AD) to precisely compute derivative information, constructing loss functions with PDE residuals, boundary conditions, and initial conditions as regularisation constraints. This mechanism approximates continuous physical fields without requiring mesh discretisation, thereby supporting both forward multi-physics simulation and inverse parameter identification based on sparse observations within a unified mathematical framework.

Within the PINN framework, deep neural networks (DNNs) serve as generalised function approximators for the physical field under investigation. For spatio-temporally dependent physical problems, the network constructs a nonlinear mapping $\mathcal{N}:\mathrm{x}\mapsto\mathrm{u}$ from spatio-temporal coordinates $\mathrm{x}=(x,y,z,t)$ to physical state variables (such as displacement u or potential ϕ).

Unlike early universal approximation theorems, modern deep learning theory focuses more on the expressive advantages brought by "depth." Yarotsky's[43] error bound theory demonstrates that for physical functions with sufficient smoothness,

deep networks can achieve equivalent approximation accuracy with far fewer parameters than shallow networks, explaining their efficiency in handling high-dimensional physical problems. Furthermore, to overcome the limitation of traditional piecewise linear activation functions like Rectified Linear Unit (ReLU)—whose second derivatives are zero, rendering them unsuitable for describing physical processes involving higher-order derivatives—PINNs typically employ smooth nonlinear activation functions such as the hyperbolic tangent function[44]. This not only ensures the continuity of physical residuals but also effectively mitigates spectral bias in high-frequency problems, providing a mathematical foundation for simulating complex force-electric coupling fields.

Although DNNs possess formidable approximation capabilities, the network itself remains physically agnostic. At this juncture, it becomes necessary to introduce PDE that comply with physical laws to physically drive the DNN, thereby constraining and guiding its behaviour. For general nonlinear PDE systems:

$$\mathcal{F}(u) = \frac{\partial u}{\partial t} + \mathcal{N}[u] - f(\mathrm{x}, t) = 0 \tag{22}$$

The key technology distinguishing it from traditional FEM lies in AD. PINN abandons mesh-based finite difference approximations. Instead, it utilises computational graphs and the chain rule to compute arbitrary-order partial derivatives of network outputs with respect to input coordinates directly at machine precision. This property confers a genuinely mesh-free nature upon PINN: it requires no laborious mesh partitioning for complex geometries such as TPMS, instead establishing physical constraints through random sampling of configuration points within the computational domain. Shin et al. [37] theoretically demonstrated that under certain conditions, this sequence based on continuous functions converges to the strong solutions of linear elliptic and parabolic PDEs, establishing the theoretical completeness of PINN as a rigorous numerical solver. The precise and efficient computational results obtained through the AD method lay the groundwork for subsequent correction of DNNs driven by loss functions.

The training process of PINN involves solving a multi-objective optimisation problem, where the total loss function is typically composed of a data matching term, a boundary condition term, and a weighted physical residual term:

$$\mathcal{L}(\theta) = w_{\text{data}}\mathcal{L}_{\text{data}} + w_{\text{PDE}}\mathcal{L}_{\text{PDE}} + w_{\text{BC}}\mathcal{L}_{\text{BC}} \tag{23}$$

Where, $\mathcal{L}_{data}$: Data matching term, used to assimilate sparse experimental observations or high-fidelity simulation solutions, formulated as mean squared error. $\mathcal{L}_{BC}$: Boundary/initial condition term, enforcing the network to satisfy Dirichlet or Neumann boundary constraints (soft constraints). $\mathcal{L}_{PDE}$: Computed physical residual term, which constitutes the core of PINN. The network continuously updates its parameters via backpropagation algorithms until the physical residual approaches zero, thereby ensuring the DNN's output satisfies the physical constraints of the PDE.

3.2 Comparison of PINN with Traditional Methods

This section aims to dissect the fundamental differences in physical representation logic between PINNs and traditional FEM alongside purely data-driven models (such as CNNs). FEM relies on geometric discretisation, with accuracy constrained by mesh quality; purely data-driven models focus on statistical mapping, exhibiting strong data dependency and lacking physical induction bias. In contrast, PINN achieves a profound integration of physical mechanisms and data observations by embedding governing equations within the loss function. The following sections elucidate PINN's unique computational advantages across three dimensions: geometric representation scalability, forward-inverse problem solving paradigms, and physical consistency. These enable PINN to overcome mesh distortion, break through the small-sample bottleneck, and achieve multi-field coupled parameter inversion.

3.2.1 Scalability of Geometric Discretisation Constraints and High-Dimensional Computation

As a standard tool in structural mechanics, the accuracy of FEM solutions is strictly constrained by the quality of mesh discretisation. While it performs reliably in two-dimensional plane problems, FEM faces severe mesh generation bottlenecks when handling complex three-dimensional topologies. Firstly, computational costs become disproportionate: to approximate smooth surfaces, the reconstruction (re-meshing) of unstructured meshes frequently consumes over 70% of the entire simulation cycle. Secondly, numerical stability risks arise, as intricate geometric features readily induce mesh distortion, subsequently triggering singular Jacobian matrices and computational divergence.

Traditional CNN models are constrained by voxelization strategies, facing computational barriers and geometric scaling effects. To overcome this bottleneck, Ren et al. [10] and Sharma et al. [11] shifted toward more efficient low-dimensional feature-driven approaches. Utilizing explicit parameter mapping (PSMNN) and graph-based representations respectively, they successfully achieved high-fidelity reconstruction of complex metamaterials within low-dimensional spaces (Fig. 3(a,b)). However, these approaches remain fundamentally data-driven. While they address the efficiency issues of geometric characterization, model training still heavily relies on massive finite element simulation labels, failing to overcome the fundamental constraint of high data acquisition costs.

By contrast, the breakthrough of PINN lies in its adoption of a continuous sampling mechanism based on coordinate points (x, y, z, t). As a mesh-free approach, the network size of PINN scales linearly with input dimensions rather than exponentially. This inherently enables PINN to circumvent geometric errors and cubic computational bottlenecks associated with mesh partitioning when handling three-dimensional solid piezoelectric metamaterials. Consequently, it achieves infinite-resolution approximations of physical fields across continuous domains at comparatively low computational expense. This characteristic naturally accommodates the implicit representation of complex structures such as TPMS[45], whilst loss function weighting facilitates multi-physics field balancing[46].

3.2.2 The Paradigm Shift in Solving Positive and Negative Problems

In the engineering applications of metamaterial design, material parameter identification and topology optimisation are often more critical than forward prediction. In this task, the solution paradigms of the three approaches exhibit fundamental differences.

Traditional FEM solutions to inverse problems inherently constitute a “black-box” optimisation process. Due to the inability to directly compute derivatives, an outer optimisation loop is typically required, involving repeated invocations of the forward solver and updates to the geometric mesh. Each parameter iteration necessitates a complete finite element simulation, and this high-frequency re-analysis leads to an exponential explosion in computational cost during multi-parameter space searches.

Although CNNs exhibit extremely rapid inference speeds, they face severe data dependency and lack of generalisation capability in inverse problems: training a high-precision inversion network requires vast amounts of ‘geometry-response’ labelled data, whose generation often still relies on costly FEM simulations due to offline data generation bottlenecks. Simultaneously, purely data-driven models merely provide statistical fits to physical laws, lacking physical constraints. Should the parameters to be inverted fall outside the distribution range of the training set, the model’s predictive capability deteriorates sharply, with no guarantee that results satisfy fundamental physical conservation laws.

PINN proposes a transformative solution paradigm: within this framework, unknown material or geometric parameters may be treated as trainable variables, updated concurrently with network weights during the same backpropagation iteration. This enables PINN to simultaneously predict forward physical fields and identify reverse constitutive parameters at the cost of a single training run. This physically driven self-supervised mechanism not only eliminates reliance on external labelled data but also significantly accelerates the iterative cycle of metamaterial design. Table 1 provides a comparative analysis of traditional finite element methods, purely data-driven neural networks, and PINN from multiple perspectives.

Table 1: Comparative analysis of FEM, CNN and PINN frameworks

Feature	Finite Element Method (FEM)	Pure Data-Driven DL (CNN)	Physics-Informed NN (PINN)
Discretization	Mesh-based (Dependent on mesh quality; prone to distortion)	Grid/Voxel-based (Limited by resolution; cubic complexity)	Mesh-free (Continuous coordinate sampling; infinite resolution)
Physics Enforcement	Intrinsic (Variational principles/Weak form)	Absent (Statistical correlation only; “Black-box”)	Constraint-based (PDE residuals embedded in loss function)
Data Requirement	Minimal (BCs & constitutive parameters only)	High (Requires massive labeled datasets from FEM/Exp)	Minimal (Physics-driven; capable of zero-shot learning)

Feature	Finite Element Method (FEM)	Pure Data-Driven DL (CNN)	Physics-Informed NN (PINN)
Scalability	Exponential (Suffers from "Curse of Dimensionality")	Cubic ($O(N^3)$) (Restricted by voxelization scaling barrier)	Linear (Scales linearly with input dimension)
Inverse Problem	Iterative Re-analysis (High cost due to re-meshing loops)	Fast Inference (Poor extrapolation beyond training data)	Unified Optimization (Parameters updated via back-propagation)
Generalization	High (Within continuum mechanics assumptions)	Low (Poor Out-of Distribution performance)	High (Guaranteed by physical laws)

3.3 Model Improvement and Evolution of PINN

Despite demonstrating considerable potential in solving general partial differential equations, standard PINNs often exhibit convergence stagnation or insufficient accuracy when confronted with the multiscale wave propagation, strongly coupled stiffness singularities, and complex periodic topologies characteristic of piezoelectric metamaterials. To address these challenges, the academic community has proposed a series of improvement strategies encompassing feature embedding, loss weighting, regional decomposition, and operator learning.

Regarding the high-frequency fluctuations and bandgap characteristics commonly observed in the dynamic analysis of piezoelectric metamaterials, standard multi-layer perceptrons (MLPs) exhibit significant spectral bias, wherein the network tends to prioritise fitting low-frequency components while neglecting high-frequency details. To overcome this limitation, Tancik et al. [47] introduced Fourier Feature Embeddings. By mapping input coordinates to a high-dimensional sinusoidal feature space, this approach substantially enhances the network's ability to resolve stress concentrations at microstructural edges and propagate short-wavelength phenomena. Building upon this foundation, the SIREN architecture employs periodic activation functions to further ensure computational accuracy for higher-order derivatives[48].

To address the parameter disparity and stiffness ill-posedness spanning up to 20 orders of magnitude between force-electric coupling fields, adaptive weighting mechanisms have been widely adopted [49]. Unlike traditional methods involving manual adjustment of fixed weights, this mechanism dynamically balances the residual contributions from the momentum equation and Maxwell's equations during training by utilising gradient statistical information. This effectively prevents numerically dominant mechanical terms from dictating the optimisation direction, thereby ensuring synchronous convergence across multiple physical fields.

When confronted with highly complex bionic topological structures such as TPMS, a single network struggles to capture global geometric features. Extended PINN and conservative PINN introduce the concept of domain decomposition [50], partitioning complex macroscopic arrays into multiple subdomains. By employing several sub-neural networks to solve problems in parallel and exchanging information through interface conditions, this approach not only reduces training complexity but also inherently aligns with the demands of high-performance parallel computing.

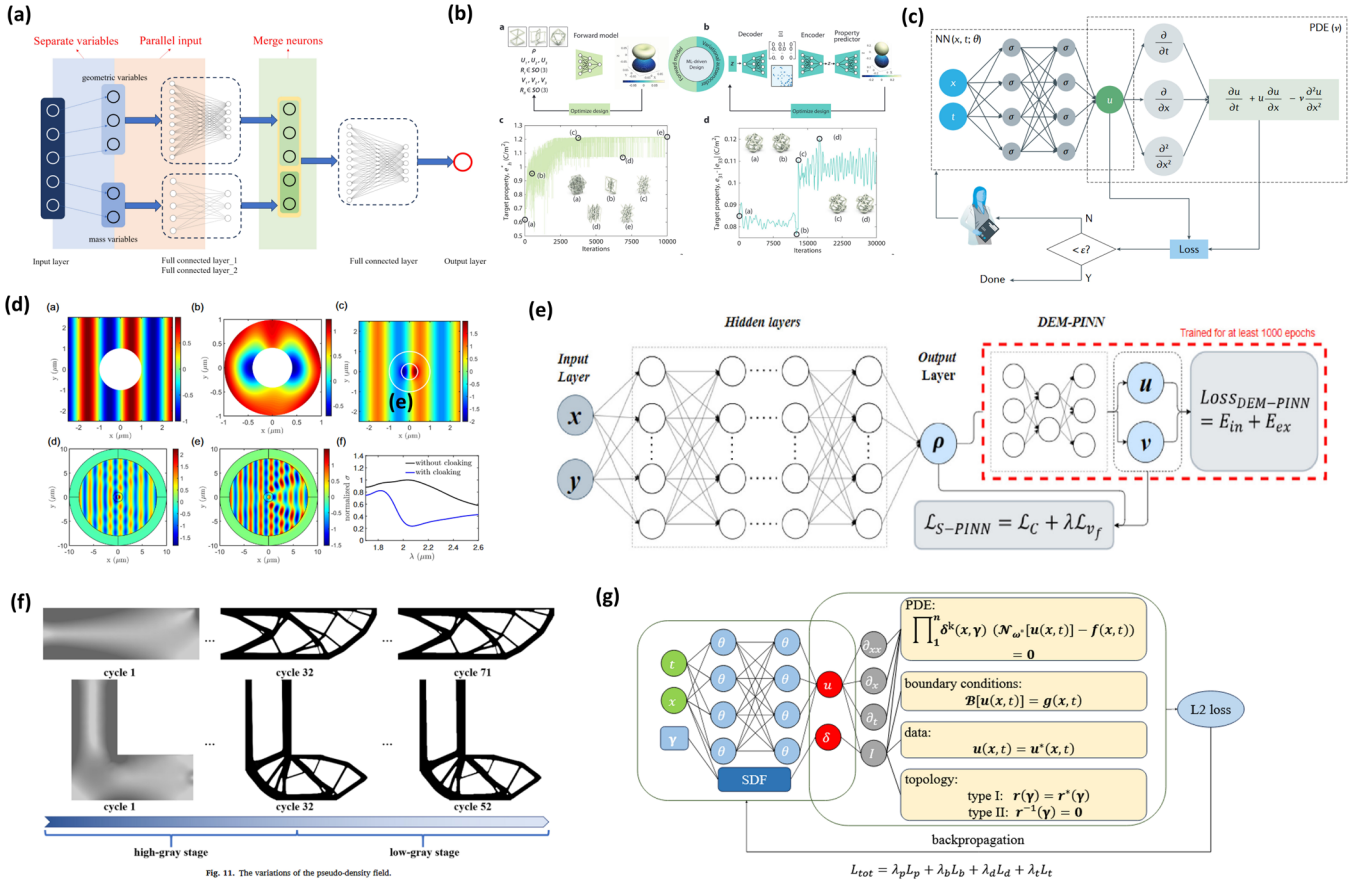
To overcome the efficiency bottleneck of PINNs' one-time training and support real-time inverse design, research focus is progressively shifting towards neural operator learning. Novel architectures such as DeepONet[51] and Fourier Neural Operators[52] no longer confine themselves to solving equations for single operating conditions, but instead strive to learn nonlinear operator mappings from microstructural parameters to macroscopic response fields. Once trained, such models enable millisecond-scale real-time inference, providing a revolutionary tool for rapid topological optimisation and parameter scanning of piezoelectric metamaterials. Table 2 summarises PINN advancements in metamaterial applications.

Table 2: Development of PINN

Year	Research Content	Key Technical Iterations	Key Progress
2020	Physics-informed neural networks for inverse problems in nano-optics and metamaterials[53]	Fundamental PINN framework, meshless inverse scattering	First determination of the effective dielectric constant for finite-size scattering systems, surpassing effective medium theory (Fig. 3(d))

Year	Research Content	Key Technical Iterations	Key Progress
2023	Recent advances in metasurface design with PINNs[54]	PINN combined with topology optimisation	Emphasising physical accuracy and computational efficiency to enhance the versatility of reverse engineering
2023	PINN for for structural topology optimization[55]	A mesh-free topology optimisation framework has been established.	The improved DEM-PINN not only enables prediction but also replaces sensitivity analysis, achieving automatic structural evolution (Fig. 3(e))
2024	Dynamically configured PINN for topology optimization[16]	Dynamic Subnet Configuration and Active Sampling	Enhance optimization efficiency, replacing finite element analysis (Fig. 3(f))
2025	PINNs for topological metamater- ial design[56]	Pre-training + Inverse Design Model + Physically Equivalent Integration	Low-frequency broadband performance, flexible waveguide manipulation, sixfold expansion of bandgap
2025	LT-PINN: Lagrangian topology-conscious PINN[57]	Lagrange Boundary Focusing + Hard Constraint	Processing multi-scale hierarchies to enhance the accuracy of complex geometries (Fig. 3(g))

Figure 3: Data-Driven frameworks and the advancement of PINNs. (a) Data-driven framework based on parallel separated multi-input neural networks (PSMNN) [10]. (b) Machine learning-based optimisation design of piezoelectric metamaterials[11]. (c) Foundational model framework of PINN[14] . (d) Scattering data framework established via PINN framework, enabling novel dielectric devices with significantly reduced scattering performance (e) Schematic of the CPINNTO architecture, where the output density of S-PINN undergoes forward propagation via the DEM-PINN loss[55] .(f) Design of advanced piezoelectric metamaterials through integrated topology and shape optimisation[16] . (g) Lagrangian Topology-Aware PINN (LT-PINN) framework for boundary-directed engineering optimisation[57].



4. Applications of PINN in Metamaterials and Multiphysics

This section broadens the perspective from pure algorithmic theory to the cutting edge of complex engineering applications. We systematically review the latest developments in PINNs for handling strong multiphysics coupling mechanisms,

constructing parametric surrogate models for metamaterials, and driving complex microstructure inverse topology optimisation. The emphasis lies in analysing how PINNs overcome the limitations of traditional FEM concerning mesh dependency and multi-field interface interpolation. We further explore the theoretical challenges and technical pathways involved in migrating these generalised multiphysics solution strategies to the domain of piezoelectric metamaterials.

4.1 Method Transfer in Multiphysics Coupling Scenarios

Prior to the extensive exploration of force-electric coupling in piezoelectric effects by PINN, this methodology had already demonstrated its unique advantages in solving classical multiphysics problems such as thermal-mechanical and fluid-structure interactions. However, this represents not a simple superposition of physical equations, but rather a fundamental shift in the underlying numerical computational paradigm.

In the classical thermo-mechanical coupling problem, the heterogeneity of physical fields already poses significant challenges. When an electric field is introduced to form a thermo-electro-mechanical three-field coupling, the complexity of the problem increases exponentially. For instance, Zhang et al. [58,59] recently demonstrated in their study of functionally graded piezoelectric plates that the nonlinear interaction between the temperature field and a strong electric field can induce highly complex dynamic responses. When addressing such multi-physics systems, traditional PINNs are highly susceptible to “Gradient Pathology” in multi-objective optimization due to the vastly different decay scales and energy levels typically exhibited by temperature, stress, and electric potential fields. To address this common challenge, recent work successfully balanced differences among control equations in transient 3D problems and large-scale ratio structures by introducing adaptive weighting strategies and mixed variable formulations [60], effectively resolving network convergence stagnation caused by stiffness mismatch (Fig. 4(b)).

In the more complex domain of fluid-structure interaction, PINN demonstrates flexibility surpassing traditional mesh-based methods. A domain decomposition framework combined with the Immersed Boundary Method has been proven capable of accurately simulating convective heat transfer and fluid stress transfer at moving interfaces [61]. Unlike traditional FEM, which is often constrained by cumbersome and error-prone data interpolation mapping between heterogeneous physical fields (e.g., fluid and solid), PINN’s continuous domain coordinate sampling eliminates this limitation entirely. As demonstrated by Rezaei et al. [62], by introducing hybrid variable formulations, PINN can directly construct and solve coupled equation systems on the same set of spatial grid points, effectively circumventing mesh compatibility issues at interfaces. This unique advantage enables the network to simultaneously approximate velocity, pressure, displacement, and potential fields within a unified coordinate system, achieving high-precision multiphysics coupling solutions without requiring mesh mapping.

This “meshless, unified coordinate system” feature holds revolutionary significance for piezoelectric metamaterial research. In piezoelectric composites, the electric field concentration effect typically occurs within an extremely narrow region at the two-phase interface, requiring extremely high-density mesh refinement in traditional FEM. PINNs, however, employ residual-driven adaptive sampling to automatically identify regions of rapid change in the electric-force coupling gradient. This approach eliminates meshing compatibility issues at multi-field interfaces, offering a novel strategy for high-fidelity simulation of interfacial polarization behavior in piezoelectric microstructures [63].

4.2 Forward prediction of metamaterial mechanical behaviour

In solving forward problems, PINN is increasingly becoming the preferred tool for constructing efficient parametric surrogate models for metamaterials. Traditional data-driven deep learning models rely on massive amounts of FEM simulation data as labels, representing “black-box” interpolation. In contrast, the PINN approach directly embeds control equations into the loss function, eliminating the need to pre-generate large discrete datasets. In the field of mechanical metamaterials, existing research has leveraged this mechanism to handle complex linear elastic and elastoplastic constitutive relations [64]. Furthermore, it has established nonlinear mappings between microscopic lattice configurations and macroscopic dispersion relations (as shown in Fig. 4(c)), enabling sub-second predictions of band structures [56].

Extending this paradigm to the field of piezoelectric metamaterials holds immense engineering value but also presents formidable computational challenges due to the high-dimensional parameter space. Unlike purely elastic media, piezoelectric response involves not only the intrinsic coupling of fourth-order elastic tensors and third-order piezoelectric tensors but is

also significantly modulated by the impedance characteristics of external shunt circuits. Under extreme operating conditions, this predictive complexity is further amplified. As demonstrated by Zhang et al.[65-67] in their recent studies on piezoelectric shells, flexible cables, and membrane structures, neglecting nonlinear constitutive relationships under the combined effects of strong electric fields and geometric nonlinearity leads to substantial errors in dynamic response prediction. Maintaining accuracy necessitates the use of computationally expensive numerical techniques. This scenario of strong nonlinear coupling, where traditional computational costs surge dramatically, powerfully underscores the urgency of developing efficient PINN-based surrogate models to achieve rapid, high-fidelity predictions.

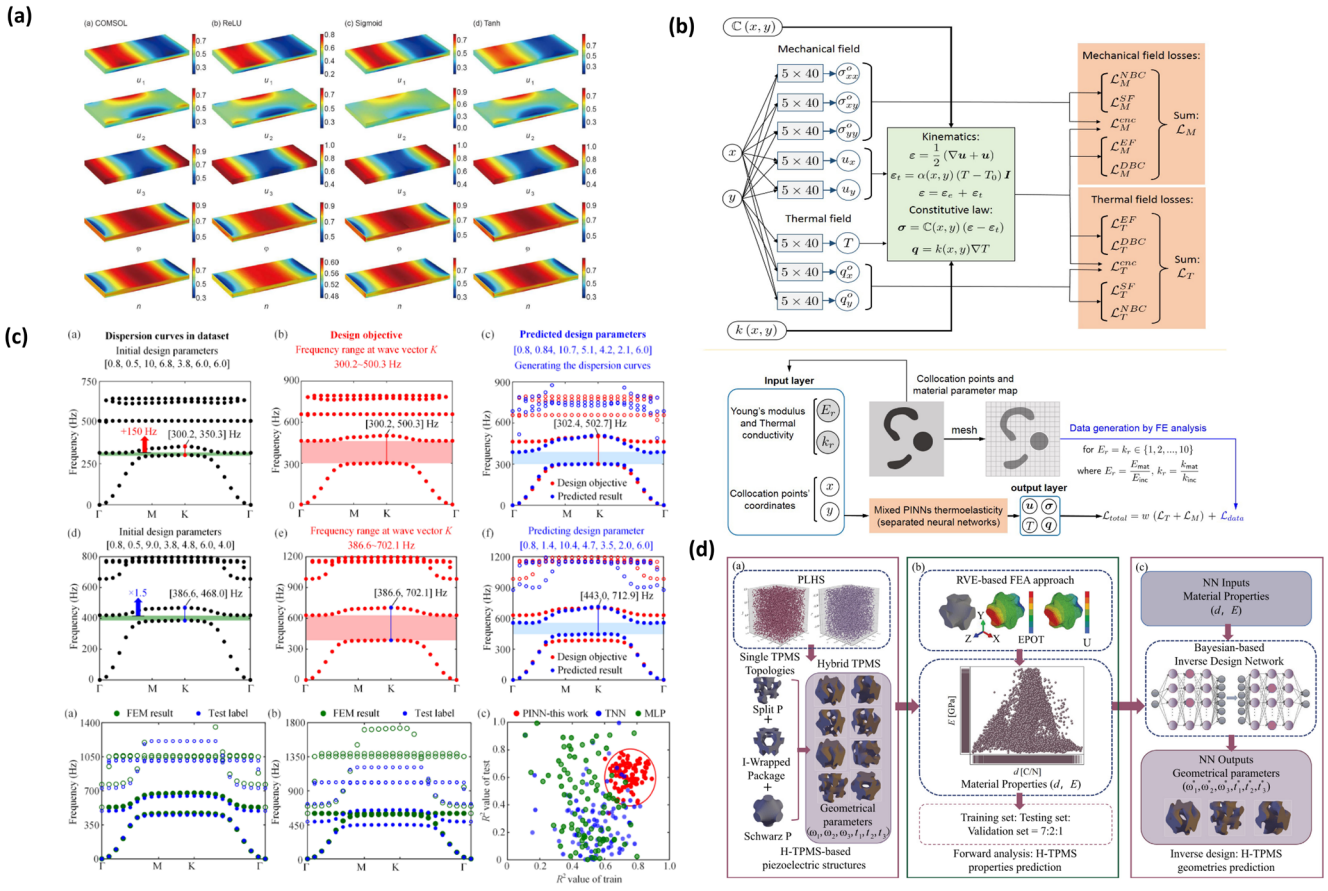
For such prediction challenges involving complex circuits and multi-field coupling, recent breakthroughs have demonstrated promising solutions. For instance, by constructing a hybrid PINN architecture incorporating circuit topology constraints, researchers successfully integrated geometric parameters, material polarization directions, and circuit loads as network inputs, achieving direct mapping to macroscopic voltage outputs or impedance spectra[68]. Similarly, in more intricate piezoelectric semiconductor studies, as illustrated in Fig. 4(a), PINN has also proven effective in tackling the nonlinear prediction challenge of the thermo-deformation-polarization-carrier (TDPC) quadruple field coupling[13], further demonstrating its exceptional generalization capability within high-dimensional multi-physics parameter spaces.

4.3 Reverse Engineering and Topology Optimisation

Reverse design, as the core approach for achieving on-demand customization of metamaterials, has long been constrained by the high computational cost of forward solutions and the difficulty in obtaining gradients. Unlike traditional Solid Isotropic Material Penalty (SIMP) or Level Set Method approaches, PINN-driven topology optimization introduces a Neural Implicit Representation mechanism. This eliminates direct dependence on discrete mesh cell density through fully connected function approximation. Within this framework, geometric evolution is reformulated as an iterative update of neural network weights. This parameterization fully leverages automatic differentiation, effectively circumventing the cumbersome sensitivity analysis inherent in traditional adjoint methods. This “meshless” or “weakly meshed” characteristic enables PINNs to drive geometric configurations to evolve autonomously within a continuous design space while satisfying control equations, thereby pioneering a novel mathematical solution pathway for structural optimization[56].

In the field of piezoelectric metamaterials, PINN demonstrates exceptional advantages, primarily manifested in its capability to solve inverse problems under multi-physics coupling constraints. Due to the bidirectional strong coupling between force and electric fields in the piezoelectric effect, traditional optimization methods often get stuck at local optima when pursuing maximization of piezoelectric coupling coefficients or sensing sensitivity in specific directions, primarily due to multi-objective conflicts and the enormous computational demands of the Jacobian matrix[69]. In contrast, PINNs can directly embed complex force-electric coupling equations as soft constraints within the loss function, enabling the network to inherently satisfy physical conservation laws while seeking optimal microstructure parameters. Although direct PINN-based topology optimization for piezoelectric metamaterial microstructures remains exploratory, pioneering work has demonstrated its immense potential for handling complex geometries[70]. Particularly for microstructures like TPMS or hierarchical structures—which exhibit outstanding piezoelectric-mechanical properties but possess complex geometries—PINN holds promise to overcome computational barriers of traditional numerical methods. It enables direct inverse derivation of optimal topologies based on target piezoelectric responses (as shown in Fig. 4(d)), providing novel mathematical tools and theoretical foundations for designing next-generation smart metamaterials with breakthrough performance metrics[71].

Figure 4: Applications of PINNs in metamaterials and multi-physics fields. (a) The high agreement between the DDPINNs-TD model based on three-dimensional theory and the COMSOL structure demonstrates its reliability under complex multi-field coupling[13]. (b) Investigation of thermal-mechanical coupling through network architecture and loss functions tailored for multi-physics problems, integrating data and physical models with transfer learning-based input and loss functions[60]. (c) Inverse design outcomes under diverse objectives demonstrated exceptional accuracy in predicting dispersion bandgaps, robustly validating its superior performance in metamaterial design[56]. (d) A deep learning-based inverse design framework offers a promising and viable approach for designing composite TPMS structures[71].



Conclusion

This paper provides a systematic review of the latest research advances in PINNs for analysing the mechanical behaviour of piezoelectric metamaterials, multi-physics coupling modelling, and topology-optimised design. By thoroughly analysing the computational bottlenecks of traditional numerical methods (such as FEM) when handling complex microstructures, alongside the generalisation limitations of purely data-driven deep learning models, we demonstrate the unique advantages of PINN as a SciML framework that integrates physical principles. This framework proves particularly effective in addressing high-dimensional, multi-field coupling, and inverse problems. Through a comprehensive review of existing literature, the principal conclusions and perspectives drawn in this paper are summarised as follows:

(1)Mesh-free properties overcome geometric complexity constraints: Unlike traditional finite element methods reliant on high-fidelity mesh partitioning, PINN employs a mesh-free solution strategy based on coordinate points. This characteristic entirely eliminates computational burdens arising from mesh distortion and reconstruction when handling complex topologies common in piezoelectric metamaterials, thereby providing a benchmark for multiphysics simulations under extreme geometric configurations.

(2)The physically embedded mechanism ensures prediction reliability: PINN successfully overcomes the issues of interpretability and physical inconsistency faced by purely data-driven models by explicitly embedding piezoelectric constitutive equations, geometric equations, and boundary conditions as regularisation terms within the loss function. Even under sparse or unlabelled data conditions, PINN ensures predictions strictly adhere to energy conservation and thermodynamic laws, significantly enhancing the model's generalisation capability.

(3)The inherent advantages of inverse problem solving and parameter identification: In the inverse design of piezoelectric metamaterials, PINN demonstrates superior robustness compared to traditional gradient-based optimisation algorithms. It enables the simultaneous optimisation of unknown material parameters or damage fields as trainable variables alongside network weights, thereby accurately identifying anisotropic parameters and microstructural defects within noisy experimental data. This achieves integrated solution for both direct and inverse problems.

(4)A marked improvement in topology optimisation efficiency: Integrating PINNs into the topology optimisation loop to construct physics-based surrogate models effectively resolves the issues of costly Jacobian matrix computations and slow iterative convergence inherent in traditional methods. This approach not only accelerates multi-objective optimisation processes but also provides real-time gradient information for designing metamaterials with specific bandgap characteristics or maximised electromechanical coupling coefficients.

In summary, the PINN framework effectively balances computational efficiency and physical fidelity by integrating physical mechanisms with data-driven approaches, thereby establishing its leading position in the analysis of piezoelectric metamaterials. To bridge the gap between theoretical modelling and engineering implementation, future research should focus on developing adaptive weighting strategies to overcome optimisation pathologies arising from multi-field coupling, whilst leveraging neural operators to address real-time inference bottlenecks in large-scale systems. With breakthroughs in these key technologies, this methodology holds promise to evolve into a robust computational strategy for tackling complex coupled problems, providing core theoretical support for the precise design of next-generation high-end intelligent equipment.

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Conflict of Interests

The authors declare that there is no conflict of interest regarding the publication of this paper.

Reference

[1] Bischof, R., & Kraus, M. A. (2025). Multi-objective loss balancing for physics-informed deep learning. Computer Methods in Applied Mechanics and Engineering, 439, 117914. https://doi.org/10.1016/j.cma.2025.117914

[2] Burbano, A., Zorin, D., & Jarosz, W. (Eds.). (2024). Data-efficient discovery of hyperelastic TPMS metamaterials with extreme energy dissipation. In Special Interest Group on Computer Graphics and Interactive Techniques Conference Conference Papers 24. ACM.

[3] Chen, K., Dong, X., Gao, P., Chen, Q., Peng, Z., & Meng, G. (2025). Physics-informed neural networks for topological metamaterial design and mechanical applications. International Journal of Mechanical Sciences, 301, 110489. https://doi.org/10.1016/j.ijmecsci.2025.110489

[4] Chen, S., Tong, X., Huo, Y., Liu, S., Yin, Y., Tan, M., Cai, K., & Ji, W. (2024). Piezoelectric biomaterials inspired by nature for applications in biomedicine and nanotechnology. Advanced Materials, 36, 2406192. https://doi.org/10.1002/adma.202406192

[5] Chen, Y., Lu, L., Karniadakis, G. E., & Dal Negro, L. (2020). Physics-informed neural networks for inverse problems in nano-optics and metamaterials. Optics Express, 28, 11618. https://doi.org/10.1364/OE.384875

[6] Danawe, H., & Tol, S. (2023). Electro-momentum coupling tailored in piezoelectric metamaterials with resonant shunts. APL Materials, 11, 091118. https://doi.org/10.1063/5.0165267

[7] Didilis, K., Selicani, G. V., Tinti, V. B., Mobin, M., Brouczek, D., Staal, L., Marani, D., Insinga, A. R., Haugen, A. B., & Esposito, V. (2026). Topology-driven electromechanical actuation in 3D-printed TPMS piezoelectric ceramics. Acta Materialia, 303, 121724. https://doi.org/10.1016/j.actamat.2025.121724

[8] Fan, G., Guo, N., Ahmed, M., & Ghazouani, N. (2025). Physics-informed neural network-enhanced simulation to estimate piezoelectric energy harvesting in cantilevered metamaterial concrete systems under wind excitation. Mechanics of Advanced Materials and Structures, 1–17. https://doi.org/10.1080/15376494.2025.2476205

[9] Fang, D., & Tan, J. (2022). Immersed boundary-physics informed machine learning approach for fluid–solid coupling. Ocean Engineering, 263, 112360. https://doi.org/10.1016/j.oceaneng.2022.112360

[10] Fang, Z., & Zhan, J. (2020). Deep physical informed neural networks for metamaterial design. IEEE Access, 8, 24506–24513. https://doi.org/10.1109/ACCESS.2019.2963375

[11] Faraci, D., Comi, C., & Marigo, J.-J. (2022). Band gaps in metamaterial plates: Asymptotic homogenization and bloch-floquet approaches. Journal of Elasticity, 148, 55–79. https://doi.org/10.1007/s10659-022-09879-3

[12] Gao, M., He, Z., Liu, J., Lü, C., & Wang, G. (2025). A dynamic homogenization method for elastic wave band gap and initial-boundary value problem analysis of piezoelectric composites with elastic and viscoelastic periodic layers. Journal of the Mechanics and Physics of Solids, 197, 106048. https://doi.org/10.1016/j.jmps.2025.106048

[13] Gao, Z., Lei, Y., Li, Z., Yang, J., Yu, B., Yuan, X., Hou, Z., Hong, J., & Dong, S. (2025). Artificial piezoelectric metamaterials. Progress in Materials Science, 151, 101434. https://doi.org/10.1016/j.pmatsci.2025.101434

[14] Guo, J., Zhu, H., Yang, Y., & Guo, C. (2025). Advances in physics-informed neural networks for solving complex partial differential equations and their engineering applications: A systematic review. Engineering Applications of Artificial Intelligence, 161, 112044. https://doi.org/10.1016/j.engappai.2025.112044

[15] Haghighat, E., Raissi, M., Moure, A., Gomez, H., & Juanes, R. (2021). A physics-informed deep learning framework for inversion and surrogate modeling in solid mechanics. Computer Methods in Applied Mechanics and Engineering, 379, 113741. https://doi.org/10.1016/j.cma.2021.113741

[16] Harandi, A., Moeineddin, A., Kaliske, M., Reese, S., & Rezaei, S. (2024). Mixed formulation of physics-informed neural networks for thermo-mechanically coupled systems and heterogeneous domains. Numerical Methods in Engineering, 125, e7388. https://doi.org/10.1002/nme.7388

[17] He, Z., Liu, J., & Chen, Q. (2023). Higher-order asymptotic homogenization for piezoelectric composites. International Journal of Solids and Structures, 264, 112092. https://doi.org/10.1016/j.ijsolstr.2022.112092

[18] Institute of Electrical and Electronics Engineers. (1988). IEEE standard on piezoelectricity. https://doi.org/10.1109/IEEESTD.1988.79638

[19] Jagtap, A. D., Kharazmi, E., & Karniadakis, G. E. (2020). Conservative physics-informed neural networks on discrete domains for conservation laws: Applications to forward and inverse problems. Computer Methods in Applied Mechanics and Engineering, 365, 113028. https://doi.org/10.1016/j.cma.2020.113028

[20] Jeong, H., Batuwatta-Gamage, C., Bai, J., Xie, Y. M., Rathnayaka, C., Zhou, Y., & Gu, Y. (2023). A complete physics-informed neural network-based framework for structural topology optimization. Computer Methods in Applied Mechanics and Engineering, 417, 116401. https://doi.org/10.1016/j.cma.2023.116401

[21] Ji, W., Chang, J., Xu, H.-X., Gao, J. R., Gröblacher, S., Urbach, H. P., & Adam, A. J. L. (2023). Recent advances in metasurface design and quantum optics applications with machine learning, physics-informed neural networks, and topology optimization methods. Light Science & Applications, 12, 169. https://doi.org/10.1038/s41377-023-01218-y

[22] Jiang, J., Wu, J., Chen, Q., Chatzigeorgiou, G., & Meraghni, F. (2023). Physically informed deep homogenization neural network for unidirectional multiphase/multi-inclusion thermoconductive composites. Computer Methods in Applied Mechanics and Engineering, 409, 115972. https://doi.org/10.1016/j.cma.2023.115972

[23] Karniadakis, G. E., Kevrekidis, I. G., Lu, L., Perdikaris, P., Wang, S., & Yang, L. (2021). Physics-informed machine learning. Nature Reviews Physics, 3, 422–440. https://doi.org/10.1038/s42254-021-00314-5

[24] Kiran, R., Nguyen-Thanh, N., Yu, H., & Zhou, K. (2023). Adaptive isogeometric analysis–based phase-field modeling of interfacial fracture in piezoelectric composites. Engineering Fracture Mechanics, 288, 109181. https://doi.org/10.1016/j.engfracmech.2023.109181

[25] Li, Z., Kovachki, N., Azizzadenesheli, K., Liu, B., Bhattacharya, K., Stuart, A., & Anandkumar, A. (2021). Fourier neural operator for parametric partial differential equations. https://doi.org/10.48550/arXiv.2010.08895

[26] Li, Z., Yi, X., Yang, J., Bian, L., Yu, Z., & Dong, S. (2022). Designing artificial vibration modes of piezoelectric devices using programmable, 3D ordered structure with piezoceramic strain units. Advanced Materials, 34, 2107236. https://doi.org/10.1002/adma.202107236

[27] Liu, C., He, Z., Lü, C., & Wang, G. (2024). Concurrent topology optimization of multiscale piezoelectric actuators. International Journal of Solids and Structures, 290, 112664. https://doi.org/10.1016/j.ijsolstr.2024.112664

[28] Liu, Y., He, H., Cao, Y., Liang, Y., & Huang, J. (2024). Inverse design of TPMS piezoelectric metamaterial based on deep learning. Mechanics of Materials, 198, 105109. https://doi.org/10.1016/j.mechmat.2024.105109

[29] Lu, L., Jin, P., Pang, G., Zhang, Z., & Karniadakis, G. E. (2021). Learning nonlinear operators via DeepONet based on

the universal approximation theorem of operators. Nature Machine Intelligence, 3, 218–229. https://doi.org/10.1038/s42256-021-00302-5

[30] McClenny, L. D., & Braga-Neto, U. M. (2023). Self-adaptive physics-informed neural networks. Journal of Computational Physics, 474, 111722. https://doi.org/10.1016/j.jcp.2022.111722

[31] Meng, C., Thrane, P. C. V., Ding, F., Gjessing, J., Thomaschewski, M., Wu, C., Dirdal, C., & Bozhevolnyi, S. I. (2021). Dynamic piezoelectric MEMS-based optical metasurfaces. Science Advances, 7, eabg5639. https://doi.org/10.1126/sciadv.abg5639

[32] Nassar, M. E., Saeed, N. A., & Nasedkin, A. (2023). Determination of effective properties of porous piezoelectric composite with partially randomly metalized pore boundaries using finite element method. Applied Mathematical Modelling, 124, 241–256. https://doi.org/10.1016/j.apm.2023.07.025

[33] Nguyen, C., Zhuang, X., Chamoin, L., Zhao, X., Nguyen-Xuan, H., & Rabczuk, T. (2020). Three-dimensional topology optimization of auxetic metamaterial using isogeometric analysis and model order reduction. Computer Methods in Applied Mechanics and Engineering, 371, 113306. https://doi.org/10.1016/j.cma.2020.113306

[34] Raissi, M., Perdikaris, P., & Karniadakis, G. E. (2019). Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations. Journal of Computational Physics, 378, 686–707. https://doi.org/10.1016/j.jcp.2018.10.045

[35] Ravanbod, M., & Ebrahimi-Nejad, S. (2024). Perforated auxetic honeycomb booster with reentrant chirality: A new design for high-efficiency piezoelectric energy harvesting. Mechanics of Advanced Materials and Structures, 31, 9857–9872. https://doi.org/10.1080/15376494.2023.2280997

[36] Ren, M., Wang, C., Moshrefi-Torbati, M., Yurchenko, D., Shu, Y., & Yang, K. (2025). Optimization of a comb-like beam piezoelectric energy harvester using the parallel separated multi-input neural network surrogate model. Mechanical Systems and Signal Processing, 224, 111939. https://doi.org/10.1016/j.ymssp.2024.111939

[37] Ren, X., Das, R., Tran, P., Ngo, T. D., & Xie, Y. M. (2018). Auxetic metamaterials and structures: A review. Smart Materials and Structures, 27, 023001. https://doi.org/10.1088/1361-665X/aaa61c

[38] Rezaei, S., Harandi, A., Moeineddin, A., Xu, B.-X., & Reese, S. (2022). A mixed formulation for physics-informed neural networks as a potential solver for engineering problems in heterogeneous domains: Comparison with finite element method. Computer Methods in Applied Mechanics and Engineering, 401, 115616. https://doi.org/10.1016/j.cma.2022.115616

[39] Roberts, A. (2024). Embed in ensemble to rigorously and accurately homogenize quasi-periodic multi-scale heterogeneous material. ANZIAM Journal, 66, 1–34. https://doi.org/10.1017/S1446181124000099

[40] Serrao, P. H., & Kozinov, S. (2024). Robust mixed FE for analyses of higher-order electromechanical coupling in piezoelectric solids. Computational Mechanics, 73, 1203–1217. https://doi.org/10.1007/s00466-023-02407-7

[41] Sharma, D., & Hiremath, S. S. (2022a). Additively manufactured mechanical metamaterials based on triply periodic minimal surfaces: Performance, challenges, and application. Mechanics of Advanced Materials and Structures, 29, 5077–5107. https://doi.org/10.1080/15376494.2021.1948151

[42] Sharma, D., & Hiremath, S. S. (2022b). Additively manufactured mechanical metamaterials based on triply periodic minimal surfaces: Performance, challenges, and application. Mechanics of Advanced Materials and Structures, 29, 5077–5107. https://doi.org/10.1080/15376494.2021.1948151

[43] Sharma, S., Ammu, S. K., Thakolkaran, P., Jovanova, J., Masania, K., & Kumar, S. (2025). Piezoelectric truss metamaterials: Data-driven design and additive manufacturing. npj Metamaterials, 1, 9. https://doi.org/10.1038/s44455-025-00009-2

[44] Shi, J., & Akbarzadeh, A. H. (2019). Architected cellular piezoelectric metamaterials: Thermo-electro-mechanical properties. Acta Materialia, 163, 91–121. https://doi.org/10.1016/j.actamat.2018.10.001

[45] Shi, J., Ju, K., Chen, H., Orsat, V., Sasmito, A. P., Ahmadi, A., & Akbarzadeh, A. (2025). Ultrahigh piezoelectricity in truss-based ferroelectric ceramics metamaterials. Advanced Functional Materials, 35, 2417618. https://doi.org/10.1002/

adfm.202417618

[46] Shin, Y., Darbon, J., & Karniadakis, G. E. (2020). On the convergence of physics informed neural networks for linear second-order elliptic and parabolic type PDEs. Communications in Computational Physics, 28, 2042–2074. https://doi.org/10.4208/cicp.OA-2020-0193

[47] Sitzmann, V., Martel, J. N. P., Bergman, A. W., Lindell, D. B., & Wetzstein, G. (2020). Implicit neural representations with periodic activation functions. https://doi.org/10.48550/arXiv.2006.09661

[48] Somnic, J., & Jo, B. W. (2022). Status and challenges in homogenization methods for lattice materials. Materials, 15, 605. https://doi.org/10.3390/ma15020605

[49] Stankiewicz, G., Dev, C., Weichelt, M., Fey, T., & Steinmann, P. (2024). Towards advanced piezoelectric metamaterial design via combined topology and shape optimization. Structural and Multidisciplinary Optimization, 67, 26. https://doi.org/10.1007/s00158-024-03742-w

[50] Sun, R., Jeong, H., Zhao, J., Gou, Y., Sauret, E., Li, Z., & Gu, Y. (2024). A physics-informed neural network framework for multi-physics coupling microfluidic problems. Computers & Fluids, 284, 106421. https://doi.org/10.1016/j.compfluid.2024.106421

[51] Tancik, M., Srinivasan, P. P., Mildenhall, B., Fridovich-Keil, S., Raghavan, N., Singhal, U., Ramamoorthi, R., Barron, J. T., & Ng, R. (2020). Fourier features let networks learn high frequency functions in low dimensional domains. https://doi.org/10.48550/arXiv.2006.10739

[52] Tandis, N., & Tandis, E. (2025). A physics-informed machine learning approach to piezoelectric plate modelling. Engineering Applications of Artificial Intelligence, 160, 111847. https://doi.org/10.1016/j.engappai.2025.111847

[53] Tassi, N., Bakkali, A., Fakri, N., Azrar, L., & Aljinaidi, A. (2021). Well conditioned mathematical modeling for homogenization of thermo-electro-mechanical behaviors of piezoelectric composites. Applied Mathematical Modelling, 99, 276–293. https://doi.org/10.1016/j.apm.2021.06.019

[54] Tran, T. V., Nanthakumar, S. S., & Zhuang, X. (2025). Deep learning-based framework for the on-demand inverse design of metamaterials with arbitrary target band gap. npj Artificial Intelligence, 1, 2. https://doi.org/10.1038/s44387-025-00001-1

[55] Wang, B., Meng, D., Lu, C., Zhang, Q., Zhao, M., & Zhang, J. (2025). Physics-informed neural networks for analyzing size effect and identifying parameters in piezoelectric semiconductor nanowires. Journal of Applied Physics, 137, 024303. https://doi.org/10.1063/5.0248278

[56] Wang, D., Dong, L., & Gu, G. (2023). 3D printed fractal metamaterials with tunable mechanical properties and shape reconfiguration. Advanced Functional Materials, 33, 2208849. https://doi.org/10.1002/adfm.202208849

[57] Wu, C., Zhu, M., Tan, Q., Kartha, Y., & Lu, L. (2023). A comprehensive study of non-adaptive and residual-based adaptive sampling for physics-informed neural networks. Computer Methods in Applied Mechanics and Engineering, 403, 115671. https://doi.org/10.1016/j.cma.2022.115671

[58] Xiao, Z., Weng, Y., Yao, W., Chen, W., & Zhang, C. (2026). Nonlinear multi-field coupling analysis of piezoelectric semiconductors via PINNs. Science China Physics, Mechanics & Astronomy, 69, 214611. https://doi.org/10.1007/s11433-025-2742-6

[59] Yang, J., Li, Z., Xin, X., Gao, X., Yuan, X., Wang, Z., Yu, Z., Wang, X., Zhou, J., & Dong, S. (2019). Designing electromechanical metamaterial with full nonzero piezoelectric coefficients. Science Advances, 5, eaax1782. https://doi.org/10.1126/sciadv.aax1782

[60] Yang, Y., Meng, J., Fan, W., Lv, J., & Xu, B. (2025). Virtual element method for piezoelasticity. Numerical Methods in Engineering, 126, e70191. https://doi.org/10.1002/nme.70191

[61] Yarotsky, D. (2017). Error bounds for approximations with deep ReLU networks. Neural Networks, 94, 103–114. https://doi.org/10.1016/j.neunet.2017.07.002

[62] Yin, J., Wen, Z., Li, S., Zhang, Y., & Wang, H. (2024). Dynamically configured physics-informed neural network in topology optimization applications. Computer Methods in Applied Mechanics and Engineering, 426, 117004. https://doi.

org/10.1016/j.cma.2024.117004

[63] Zhang, Y., Huang, Y., Zhao, S., Jiao, Z., Lü, C., & Yang, J. (2025a). Nonlinear dynamic response and stability of piezoelectric shells with piezoelectric nonlinearities. International Journal of Mechanical Sciences, 304, 110731. https://doi.org/10.1016/j.ijmecsci.2025.110731

[64] Zhang, Y., Zhu, H., Zhao, S., Ni, Z., Lü, C., & Yang, J. (2025b). Nonlinear dynamic response of functionally graded plates with piezoelectric nonlinearity. European Journal of Mechanics - A/Solids, 114, 105776. https://doi.org/10.1016/j.euromechsol.2025.105776

[65] Zhang, Y., Guo, X., Wu, Y., Zhang, Y. Y., & Lü, C. (2025c). Active control of cables with piezoelectric actuation considering geometric and material nonlinearities. Engineering Structures, 340, 120773. https://doi.org/10.1016/j.engstruct.2025.120773

[66] Zhang, Y., Guo, X., Wu, Y., Zhang, Y. Y., Zhang, H., & Lü, C. (2024a). Nonlinear thermo-electro-mechanical responses and active control of functionally graded piezoelectric plates subjected to strong electric fields. Thin-Walled Structures, 205, 112375. https://doi.org/10.1016/j.tws.2024.112375

[67] Zhang, Y., Guo, X., Wu, Y., Zhang, Y. Y., Zhang, H., & Lü, C. (2024b). Vibration control of membrane structures by piezoelectric actuators considering piezoelectric nonlinearity under strong electric fields. Engineering Structures, 315, 118413. https://doi.org/10.1016/j.engstruct.2024.118413

[68] Zhang, Z., Lee, J.-H., & Gu, G. X. (2022). Rational design of piezoelectric metamaterials with tailored electro-momentum coupling. Extreme Mechanics Letters, 55, 101785. https://doi.org/10.1016/j.eml.2022.101785

[69] Zhao, W., Hao, R., Zhang, M., Chen, Q., Yang, Z., & Chen, X. (2025). Physically informed neural networks for homogenization and localization of composites with periodic microstructures. Composite Structures, 367, 119260. https://doi.org/10.1016/j.compstruct.2025.119260

[70] Zhou, L., Geng, J., Chen, P., Zhu, H., Tian, H., & Liu, X. (2024). Mechanic-electric coupling cell-based smoothed isogeometric analysis for the static behaviors of piezoelectric structures. Acta Mechanica, 235, 2803–2821. https://doi.org/10.1007/s00707-024-03856-8

[71] Zhou, Y., Wang, Z., Zhou, K., Tang, H., & Li, X. (2025). LT-PINN: Lagrangian topology-conscious physics-informed neural network for boundary-focused engineering optimization. https://doi.org/10.48550/arXiv.2506.06300