



EDITORIAL

Guest Editorial for the Special Issue on Advanced Computational Modeling and Simulations for Engineering Structures and Multifunctional Materials: Bridging Theory and Practice

S. M. Anas^{1,*} and Rayeh Nasr Al-Dala'ien^{2,*}

¹Department of Civil Engineering, Jamia Millia Islamia (A Central University), New Delhi, India

²Civil Engineering Department, College of Engineering, Al-Balqa Applied University (BAU), Salt, Jordan

*Corresponding Authors: S. M. Anas. Email: mohdanas43@gmail.com; Rayeh Nasr Al-Dala'ien. Email: Rayah.nasr1@bau.edu.jo

Received: 02 March 2026; Accepted: 16 April 2026; Published: 08 May 2026

1 Introduction

The growing use of computational modelling, simulation tools, and data-driven methods has changed the way engineering structures and advanced materials are studied and designed. With the increasing availability of high-performance computing, artificial intelligence, and multi-scale simulation techniques, computational modelling is no longer limited to purely theoretical studies. It has now emerged as a practical design aid, allowing researchers to predict material behavior, understand complex interactions, and support engineering decisions across different material and structural scales. These developments have helped in narrowing the gap between theoretical studies and practical engineering applications.

The special issue titled “Advanced Computational Modeling and Simulations for Engineering Structures and Multifunctional Materials: Bridging Theory and Practice” was published in the journal “Computers, Materials & Continua” (Tech Science Press) and was jointly edited by two Guest Editors, Dr. S. M. Anas and Dr. Rayeh Nasr Al-Dala'ien. The call for papers opened on 24 June 2024 and closed on 30 November 2025. During this period, 65 manuscripts were received from researchers across different countries, reflecting the increasing global interest in computational mechanics and material simulations. After a thorough peer-review process, seven papers were accepted, giving an overall acceptance rate of nearly 11%.

For this special issue, the Guest Editors invited contributions from researchers, academicians, industry professionals, and subject experts working in related areas. The intention was to bring together high-quality research from diverse perspectives. The response from the research community was positive, resulting in a focused collection of articles that successfully links theoretical concepts with practical applications.

The selected papers clearly indicate that computational approaches have become an essential part of modern materials and structural research. The topics span inverse modelling in anisotropic elasticity, hybrid metaheuristic and deep learning frameworks for dielectric optimization, ANN-based prediction of hybrid composite behavior, and multi-objective modelling of mechanical and damping characteristics. Other contributions address multi-scale simulation with experimental validation of nanofiller-based Polydimethylsiloxane (PDMS) sensors, AI-assisted prediction of tool wear in glass-fiber reinforced polymer (GFRP) drilling, and mesoscale finite element modelling of rubberized concrete.

The published articles [1–7] reflect the central aim of this special issue, which is to bring theory and practice closer through advanced computational methods. They show that the combined use of numerical modelling, experimental work, and intelligent algorithms offers a dependable path towards innovation and sustainable engineering solutions. This special issue not only presents valuable research outcomes but also provides insight into the future direction of computational mechanics and multifunctional materials.

2 Articles Included in the Special Issue

Hematiyan (2025) [1] introduced a boundary-type inverse method based on the Method of Fundamental Solutions (MFS) to identify unknown traction distributions on part of the boundary in two-dimensional anisotropic elastic solids. The work addressed a long-standing gap, as boundary condition identification in anisotropic materials had not received much attention earlier. The study specifically focused on traction identification in anisotropic elasticity using an inverse MFS framework, without relying on comparisons to other previously published methods. The method formulation, implementation, and validation were fully developed within the scope of this work itself. Though inverse problems related to boundary conditions in general elasticity problems have been explored in literature, this study clearly emphasized that such investigations for anisotropic traction estimation are still very limited. Hematiyan (2025) [1] modelled the problem by expressing unknown traction as a set of parameters and determining them through sensitivity analysis using multiple MFS-based direct solutions. This avoided both domain discretization and complex numerical integration [1]. Numerical examples on anisotropic materials with intricate geometries showed that strain-based data produced higher accuracy than displacement-based data [1]. Measurements taken closer to the unknown boundary improved solution stability, and accuracy improved with more measurements up to a certain limit [1]. The study also examined the influence of measurement error, location of measurement points, and number of measurements on the inverse solution accuracy. The study effectively established MFS as a dependable inverse modeling tool for traction estimation in anisotropic materials and broadened the scope of boundary-type meshless methods for such problems [1]. Results confirmed that the proposed inverse approach is efficient, stable, and capable of providing accurate traction identification even under practical measurement conditions.

In another recent work, Wang et al. (2025) [2] carried out an experimental and data-driven study to explore the relationship between composition and properties of $\text{Na}_{1/2}\text{Bi}_{1/2}\text{TiO}_3$ -based $(1-x)$ NBBT8- x BMT ceramic capacitors. They used a Cuckoo Search-Deep Neural Network (CS-DNN) framework combined with experimental measurements to optimize the material composition under uncertainty. Ceramic samples with different BMT ratios ($x = 0-0.80$, with selected compositions such as 0, 0.02, 0.04, 0.06, 0.10, 0.12, 0.14, 0.20 and 0.40) were produced through solid-state reaction, and their structural and electrical characteristics were analyzed using XRD, SEM, and dielectric-ferroelectric testing. A total of 45 data points were used to train and validate the CS-DNN model, supported by Monte Carlo sampling under a “ 3σ ” criterion [2]. Results showed that BMT addition weakened long-range ferroelectric order, lowered coercive field and remnant polarization, and reduced dielectric loss while enhancing high-temperature stability and energy storage performance [2]. The best composition (0.88NBBT-0.12BMT) achieved a discharge energy density of about 2.01 J cm^{-3} at 150 kV cm^{-1} and 120°C , with over 60% efficiency [2]. Embedding Cuckoo Search in DNN training helped the model escape local minima and provided tighter prediction ranges, with ϵ_{max} R^2 improving from 0.9382 to 0.9717 [2]. The MC/ 3σ approach gave 99.7% confidence intervals within the tested composition range. The study also highlighted challenges such as the small dataset, bimodal data distribution, and limited generalization or reliability beyond the composition range of $x = 0.80$. The authors of this published paper [2] finally demonstrated an effective uncertainty-aware framework for optimizing lead-free dielectric ceramics and suggested future extension towards larger datasets, multi-feature inputs, and improved model generalization for advanced material design.

Further, Bhat et al. (2025) [3] worked on predicting water absorption in nanoclay-modified glass fiber/epoxy composites using an Artificial Neural Network (ANN) model. Laminates were prepared with varying glass fiber (40–60 wt.%) and nano clay (0–4 wt.%) contents using hand lay-up and compression molding. These samples were immersed in water for 70 days as per ASTM D570 standard to measure absorption. Findings revealed that higher glass fiber and nano clay contents reduced water uptake because of better barrier characteristics arising from the nano clay's platelet structure and high aspect ratio, which delayed diffusion [3]. The ANN used a 3-4-1 feedforward structure with soaking time, fiber fraction, and nano clay content as inputs and water absorption as the output. Trained with the Levenberg-Marquardt algorithm, the model achieved $R = 0.998$ and a very low mean squared error (1.38×10^{-4}) [3]. Experimental validation showed a prediction error within a very small acceptable range, confirming reliability. This work [3] established that nano clay and fiber content work together to improve moisture resistance, and ANN-based modeling offers a quick, dependable method compared to extensive experiments. The study also demonstrated that the developed ANN model can effectively capture the nonlinear relationship between material composition and water absorption behavior.

Hariharan et al. (2026) [4] performed an integrated study combining Response Surface Methodology (RSM) and ANN to predict and optimize mechanical and damping properties of cast-iron (CI)-granite-epoxy (G-E) hybrid composites. The team prepared a total of 24 experimental datasets by varying epoxy, granite, and CI filler weight percentages. Tests measured compressive, tensile, and flexural strengths, elastic moduli, density, and damping behavior using ASTM-standard mechanical testing and impact hammer-based vibration analysis [4]. ANN trained with Bayesian Regularization and Levenberg-Marquardt algorithms showed that Bayesian Regularization provided more stable and reliable predictions, with average R^2 values exceeding 0.99 across most mechanical properties [4]. However, prediction accuracy for damping behavior was comparatively lower and showed higher variability, indicating the complex nature of energy dissipation mechanisms [4]. RSM provided better interpretability of factor interactions but showed lower predictive capability for certain responses, especially compressive strength and damping ratio. Granite fraction emerged as the main factor affecting performance, epoxy acted as a binder, and CI filler improved stiffness and damping at lower concentrations (around 5–10 wt%) but showed diminishing or adverse effects at higher contents due to possible agglomeration and brittleness [4]. The optimized composition indicated that moderate granite content (around 50–75 wt%) with balanced epoxy and controlled CI addition resulted in improved mechanical performance, while damping behavior depended strongly on interfacial interactions and material composition balance. The study [4] demonstrated a combined RSM-ANN framework as an effective and efficient approach for predicting and optimizing hybrid composite performance, particularly for vibration-sensitive engineering applications, while also highlighting the advantage of ANN in capturing nonlinear material behavior with limited experimental data.

Gautam et al. (2026) [5] carried out a detailed multi-scale study on PDMS-based porous capacitive pressure sensors reinforced with graphene nanoplatelets (GnP) and carbon nanotubes (CNT). The researchers [5] used a sugar-template method to create tunable porous PDMS foams by controlling sugar particle size and packing, enabling adjustable porosity and compressibility. Samples were fabricated with low filler concentrations (0.1–0.5 wt%) and cured under controlled conditions using vacuum-assisted processing. Mean-field homogenization was used to estimate effective conductivity tensors, which matched experimental I–V data showing stable Ohmic behavior [5]. These properties were further used in COMSOL 3D models to simulate diaphragm deflection, electric-field distribution, and capacitance variation under applied force in the range of 0–7 N [5]. GnP-PDMS sensors performed better, showing sensitivity of $\approx 0.032 \text{ pF}\cdot\text{N}^{-1}$, compared to CNT-PDMS ($\approx 0.019 \text{ pF}\cdot\text{N}^{-1}$) [5], and also exhibited lower hysteresis ($\sim 12.5\%$) compared to CNT-based sensors ($\sim 18\%$), indicating better elastic recovery. The advantage was linked to better GnP dispersion and

larger effective surface area, which promoted improved conductive network formation. The sensors were also tested for durability under cyclic loading, showing stable and repeatable response behavior, and were further evaluated in an insole model using finite element analysis in ABAQUS to simulate stress distribution during different gait phases (heel, mid-stance, and toe-off) [5]. This published study [5] effectively linked nano-scale material characteristics with macro-scale sensing performance and demonstrated that GnP-PDMS foam sensors provide higher sensitivity, better stability, and improved reliability for wearable pressure sensing and gait monitoring applications.

Rao et al. (2026) [6] explored tool wear behavior during dry drilling of glass-fiber reinforced polymer (GFRP) laminates. A detailed experimental plan was executed with a full factorial design consisting of 81 experiments (including replications) covering different spindle speeds, feed rates, and drill diameters. Each test used a fresh HSS drill, and average flank wear was measured after drilling 80 holes using a toolmaker's microscope. ANOVA results identified spindle speed as the key factor (74.43% influence), followed by feed rate (15.80%) and drill diameter (6.16%) with all parameters showing statistical significance ($p < 0.001$). While a linear regression model gave good accuracy ($R^2 = 96.40\%$), it struggled to capture nonlinear patterns. Hence, a multilayer feedforward ANN (3-10-6-1) was trained using the Levenberg-Marquardt algorithm [6]. The ANN achieved $R^2 \approx 0.9583$ and RMSE ≈ 0.00662 mm, with MAPE of only 2.27%, and the predictions were further validated using independent confirmation experiments showing all errors within acceptable limits. Microscopic examination confirmed abrasion, edge rounding, and microchipping as the dominant wear mechanisms. This published article [6] proved that ANN models better capture complex nonlinear behavior and serve as reliable soft computational tools for tool-condition monitoring, process optimization, and sustainable machining applications.

Lastly, Kamel et al. (2026) [7] took a numerical route to study how rubber content, particle size, and specimen dimension affect the mechanical performance of crumb rubber concrete (CRC). Using the Base Force Element Method (BFEM), a mesoscale model was created with aggregates as polygons and rubber as circular inclusions, including five distinct material phases (coarse aggregates, mortar, rubber particles, and two types of interfacial transition zones). Simulations were performed for varying rubber contents (0%–30% replacement), particle sizes (2 and 4 mm), and specimen sizes (100, 150, and 300 mm), and results were validated using available reference data within the study [7]. It was observed that higher rubber content reduced both tensile and compressive strengths by up to about 55% and 56%, respectively, at 30% rubber content. Smaller rubber particles caused greater strength reduction than larger ones, due to higher surface area and weaker interfacial zones, which increased susceptibility to micro-crack initiation. Larger specimens also showed lower strength, indicating strong size effects, with strength reductions reaching around 27.7% for larger specimens compared to smaller ones. Crack patterns revealed that damage initiated mainly in rubber-rich regions and interfacial transition zones (ITZ), and propagated through these weak zones leading to final failure. The study [7] recognized simplifications like two-dimensional mesoscale modelling and idealized circular rubber particle representation as limitations and recommended future work involving three-dimensional modelling and more realistic particle geometries for improved predictive accuracy.

3 Conclusion

This special issue in the journal “*Computers, Materials & Continua* (Tech Science Press)” presents a well-balanced set of studies that connect theoretical understanding with real-world engineering practice through computational modelling, data-driven simulation, and experimental validation. The selected papers cover a broad range of themes, including inverse mechanics, AI-based material design, hybrid composite modelling, sensor simulation, machining analysis, and mesoscale modelling of concrete systems. Each contribution

demonstrates how integrating physics-based models with data-driven techniques can improve prediction accuracy, reduce experimental effort, and accelerate innovation in materials and structural engineering.

This collection clearly shows that computational research is no longer confined to numbers and algorithms; rather, it serves as a critical link between theory, laboratory experiments, and practical engineering applications.

The Guest Editors sincerely acknowledge the efforts of all authors and reviewers for their careful and timely contributions, which have significantly strengthened this special issue. Dr. S. M. Anas served as the Lead Guest Editor and coordinated the overall editorial process of this special issue. Appreciation is also extended to the Editor-in-Chief, editorial board members, journal manager, and production team for their continuous support and attention throughout the publication process.

“May future research continues to weave theory, computation, and experiment into innovations that redefine the very fabric of materials and structures.”

With best wishes for continued endeavors that push the frontiers of knowledge.—**Dr. S. M. Anas, Lead Guest Editor**

Acknowledgement: The Guest Editors sincerely thank all authors for their valuable contributions and the reviewers for their timely and constructive feedback. Special appreciation is extended to the editorial team for their continuous support. We also acknowledge the leadership and efforts of the Lead Guest Editor, Dr. S. M. Anas, in successfully coordinating this special issue.

Funding Statement: The authors received no specific funding.

Author Contributions: The authors confirm their contribution to this editorial as follows: conceptualization, overall planning, and primary development of the special issue: S. M. Anas; co-conceptual support: Rayeh Nasr Al-Dala'ien; coordination with the journal, framing of the editorial theme, and major role in structuring the editorial: S. M. Anas; preparation and drafting of the manuscript: S. M. Anas; review of the manuscript and providing general inputs: Rayeh Nasr Al-Dala'ien. The peer review process for the manuscripts included in this special issue was carried out with the support of the journal's editorial office and editorial team in accordance with the journal policies. The final decisions on the manuscripts were approved by the Lead Guest Editor (S. M. Anas), and the Editor-in-Chief. Both authors reviewed and approved the final version of the manuscript.

Availability of Data and Materials: Not applicable.

Ethics Approval: Not applicable.

Conflicts of Interest: The authors declare no conflicts of interest.

References

1. Hematiyan MR. A boundary-type meshless method for traction identification in two-dimensional anisotropic elasticity and investigating the effective parameters. *Comput Mater Contin.* 2025;82(2):3069–90. doi:10.32604/cmc.2025.060067.
2. Wang S, Liang Y, Huang L, Li P. Cuckoo search-deep neural network hybrid model for uncertainty quantification and optimization of dielectric energy storage in $\text{Na}_{1/2}\text{Bi}_{1/2}\text{TiO}_3$ -based ceramic capacitors. *Comput Mater Contin.* 2025;85(2):2729–48. doi:10.32604/cmc.2025.068351.
3. Bhat A, Katagi NN, Gowrishankar MC, Shettar M. Prediction of water uptake percentage of nanoclay-modified glass fiber/epoxy composites using artificial neural network modelling. *Comput Mater Contin.* 2025;85(2):2715–28. doi:10.32604/cmc.2025.069842.

4. Hariharan G, Vinyas, Chennegowda GM, Kumar N, Kumar S, Doreswamy D, et al. Data-driven prediction and optimization of mechanical properties and vibration damping in cast iron-granite-epoxy hybrid composites. *Comput Mater Contin.* 2026;86(3):19. doi:10.32604/cmc.2025.073772.
5. Gautam R, Marriwala N, Devi R, Arya DS. Multi-scale modelling and simulation of Graphene-PDMS and CNT-PDMS flexible capacitive pressure sensors for enhanced sensitivity. *Comput Mater Contin.* 2026;87(2):11. doi:10.32604/cmc.2026.076136.
6. Udupi SR, Bolar G, Shettar M, Bhat A. Artificial neural network-based prediction and validation of drill flank wear in GFRP machining for sustainable and smart manufacturing. *Comput Mater Contin.* 2026;87(3):33. doi:10.32604/cmc.2026.078574.
7. Kamel MMA, Fu Y, Abeer SZ, AL-Delfi ZM, Peng Y. Numerical mesoscale analysis of rubber size, rubber content, and specimen size effects on crumb rubber concrete using BFEM. *Comput Mater Contin.* 2026;87(3):40. doi:10.32604/cmc.2026.078775.