AI in Computational Mechanics and Engineering Sciences

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Artificial Intelligence (AI) approaches have been widely used during the last two decades for different purposes and have remained a highly-researched topic, especially for complex real-world problems. On this basis, the main theme of this special issue is dedicated to developments of AI methods that give a new light to solving problems deemed difficult in Computational Mechanics and Engineering Sciences.

The paper by Yuan Feng et al., [1] titled "Stochastic nonlocal damage analysis by a machine learning approach," proposes a framework for quasi-brittle materials' nonlocal stochastic damage analysis using machine learning. A unified framework for safety assessment is developed under various working conditions to analyze and incorporate uncertain parameters of the system, including material properties and loading actions. The framework comprises a new machine-learning technique called C-X-SVR, which is implemented within the CAE platform for stochastic damage analysis. An explicit regression function representing the inherent relationship between random systematic inputs and output response can be used to solve the stochastic damage analysis of complex governing equations. This is done by developing an uncertainty quantification approach to be used in probabilistic damage problems. Consequently, real-life engineering products can be evaluated against frequently updated information for rapid uncertainty quantification. Numerical examples and experimental validation have demonstrated that the proposed framework is effective and computationally efficient [1].

The paper by Liwei Wang et al., [2] titled "Deep generative modeling for mechanistic-based learning and design of metamaterial systems," exploits data-driven metamaterials to propose a deep generative metamaterial design framework based on. A variational autoencoder (VAE) is simultaneously trained on an extensive metamaterial database to establish a map from complex microstructures into a continuous, organized, and low-dimensional latent space. A distance metric and natural interpolation method are used to encode complex shapes in latent space to measure shape similarity. Using this metric, it is possible to interpolate between microstructures and encrypt meaningful variation patterns in geometry and properties. These insights led into proposing systematic methods for designing microstructures, graded families, and multiscale systems are proposed. Two systems that achieve desired distortion behavior, i.e., heterogeneous and functionally graded metamaterial, were designed to validate the proposed framework's effectiveness [2].

The paper by Sourav Saha et al., [3] titled "Hierarchical Deep Learning Neural Network (HiDeNN): An artificial intelligence (AI) framework for computational science and engineering," uses Hierarchical Deep Learning Neural Networks (HiDeNN to develop a unified framework for solving demanding engineering and computational science problems featuring scant or no physics. The flexibility of HiDeNN is demonstrated by elaborating on construction details and mathematical elements. Three examples were solved to demonstrate the framework's accuracy, versatility, and efficiency. Results indicate HiDeNN can be applied to a class of computational mechanics problems with non-uniform microstructures at the macroscale, such as functional gradient alloys. As a result of the success of HiDeNN in solving these problems, a similar framework may be applicable to other fields where explicit physics is lacking. This may be the case with additive manufacturing [3].

The paper by Kun Wang et al. [4] titled “A non-cooperative meta-modeling game for automated third-party calibrating, validating and falsifying constitutive laws with parallelized adversarial attacks,” presents a logical approach to evaluating high-regret high-risk engineering problems using concepts adopted from machine learning and game theory techniques. A meta-modeling game involving competing AI agents has been proposed in which two AI agents calibrate and explore a given constitutive model by generating experimental data to improve experimental design and model robustness. As such, both agents can continuously improve their knowledge of the constitutive law using experimental data generated by the competitor agent in a deep reinforcement learning framework. Furthermore, they can develop Nash equilibrium strategies that provide information about the quality of the models in the decision trees. There is a wide range of applications for the developed meta-modeling game using adversarial attacks on models created by machine learning and human [4].

The paper by Kailai Xu and Eric Darve [5], titled “Solving inverse problems in stochastic models using deep neural networks and adversarial training,” proposes a novel method for estimating unknown distributions using simulated and observed random processes exhibiting the same statistical properties. To approximate the unknown distribution, neural networks are utilized as expressive tools. Next, statistical disagreements between simulated and observed processes are calculated by using a discriminative neural network. Numerical models demonstrate the method’s effectiveness at estimating the model parameters and learning complicated unknown distributions. Models using numerical data demonstrate the method's effectiveness for estimating parameter estimates and learning complex unknown distributions. Various optimization algorithms were benchmarked, and L-BFGS-B was found to have promising performance for engineering applications [5].

The paper by Giovanis and Shields [6], entitled "Data-driven surrogates for high dimensional models using Gaussian process regression on the Grassmann manifold" deals with a machine learning method for constructing a surrogate model in the context of uncertainty quantification for physical/engineering systems. A surrogate model on the parameter space of the solution of the computational model is represented on a lower-dimensional Grassmannian manifold. The construction is carried out using solution clustering and a local Gaussian process regression model, which maps the points in the parameter space to the reduced solution in the tangent space of the Grassmannian in order to predict the solution at new points in the parameter space. Two examples illustrate the methodology, which gives validation. The first example is a nonlinear three-dimensional set of stochastic ordinary differential equations subjected to random initial conditions. The second example deals with the plastic deformation of an amorphous solid using the shear transformation zone theory of plasticity [6].

"Modeling, simulation and machine learning for rapid process control of multiphase flowing foods" by Kim, Zohdi, and Singh [7] presents a model and a machine learning approach for the real-time control of the heat treatment of multiphase fluids that consist of fluidized binder materials with embedded particles. This context is that of the food industry, which desires to have a faster throughput for large-scale food production. The model developed is based on induction heating and the pressure gradient needed in the pipes to heat such multiphase materials to a target temperature and transport them with a prescribed flow rate. The optimization problem is solved with a genetic algorithm. Since fast numerical calculations must be carried out, a machine learning technique is applied to predict the fouling rate of the channel at the final processing time [7].

"A robust solution of a statistical inverse problem in multiscale computational mechanics using an artificial neural network" by Pled, Desceliers, and Zhang [8] is a paper devoted to the statistical identification of the apparent elastic properties of heterogeneous materials with complex random microstructure. A prior probability model of the random compliance elasticity field depending on hyperparameters is introduced. A neural network-based identification method is presented for solving the statistical inverse problem related to the statistical identification of the hyperparameters. Conditioning of the initial database allows for obtaining an efficiently trained neural network. A probabilistic model of the input random vector is proposed to take into account experimental errors on the network input and to perform a robustness analysis of the network output with respect to the input uncertainties level. The proposed identification method is successfully applied to real experimental data coming from experimental measurements on a cortical bone specimen [8].

The paper by Kalogeris and Papadopoulos [9], entitled "Diffusion maps-aided Neural Networks for the solution of parametrized PDEs" deals with the construction of surrogate models for stochastic solutions of parameterized random boundary value problems using neural networks and diffusion maps. The parameterized stochastic computational model is obtained by finite element discretization. The diffusion-maps basis is used as an alternative to the PCA basis to compute a reduced set of solutions. The reduction allows an efficient training of a feed-forward neural network to be obtained. The methodology is tested on two examples. The first one is the nonlinear Burger equation with random viscosity and deterministic initial and boundary conditions. The second example is a convection-diffusion-reaction equation with random coefficients, deterministic boundary conditions and zero initial condition. The results obtained validate the expected efficiency and accuracy [9].

The paper by Cortiella, Park, and Doostan [10] entitled “Sparse identification of nonlinear dynamical systems via reweighted l_1-regularized least squares” is devoted to the improvement of the accuracy and robustness of the sparse identification of nonlinear dynamics approach in presence of state measurement noise. A reweighted l_1-regularized least squares solver is developed, wherein the regularization parameter is selected from the corner point of a Pareto curve in order to better promote sparsity in the recovery of the governing equation. This method allows for mitigating the effect of noise in the state variables. A method to recover single physical constraints from state measurements is also presented. Five low-dimension nonlinear dynamical systems are analyzed to assess the performance of the proposed methodology: the Lorenz system made up of three coupled first-order equations, the Duffing oscillator, the Van der Pol oscillator, a single degree of freedom spring-mass system, and finally, the three equations of the Euler rigid body dynamics. The obtained results demonstrate the accuracy and robustness of the proposed strategy with respect to state measurement noise, thus illustrating its viability for a wide range of potential applications [10].

In their paper “Towards blending Physics-Based numerical simulations and seismic databases using Generative Adversarial Network,” Gatti and Clouteau [11] propose a methodology to mix high-fidelity physics-based models with machine learning techniques based on Generative Adversarial fully-convolutional deep neural networks. The main ideas involve finding reduced-dimensional nonlinear representations of both synthetic and experimental data, and then training a stochastic generator of fake experimental responses conditioned by the physics-based simulation results. The method is applied to the generation of broadband seismic signals by blending the low-frequency outcome of physics-based numerical simulations and broadband ground motion databases [11].

Patel, Trask, Wood, and Cyr [12] describe a new method for discovering continuum models from high-fidelity molecular simulation data in their paper “A physics-informed operator regression framework for extracting data-driven continuum models.” They assume that the dynamics can be described by a neural network parameterizing a pseudo-differential operator in modal space as well as a network parameterizing a pointwise nonlinear operator in physical space. These parameterizations allow for simple introduction of physically motivated inductive biases. The authors demonstrate that the method can recover the heat equation and fractional heat equation from density measurements of Brownian motion and Levy flight trajectories in 1D and 2D. Moreover, the method can discover models that extrapolate beyond the dynamics present in the training set [12].

Yin, Zheng, Humphrey, and Karniadakis [13] employ a novel application of physics-informed neural networks (PINNs) to biological materials in their paper “Non-invasive inference of thrombus material properties with physics-informed neural networks.” They model the thrombus as a porous medium and study its interaction with blood flow using the Cahn-Hilliard and Navier-Stokes equations. These equations are encoded into the loss functions associated with the PINNs, which serve to constrain the weights and biases of the network outputs. The method uses automatic differentiation to calculate the 4^{th} derivative in the Cahn-Hilliard equations and introduces an auxiliary network to approximate the 2^{nd} derivative of the energy potential term. The PINNs can infer hundreds of parameters based only on measurements with a limited number of training points and without any prior knowledge of the unknown parameters. The authors demonstrate the potential of PINNs to infer permeability and viscoelastic modulus from synthetic data [13].

In their paper “Data-driven learning of nonlocal physics from high-fidelity data,” You, Yu, Trask, Gulian, and D’Elia [14] propose a new way to extract nonlocal models from data, avoiding the mathematical complexity of deriving them from first principles. Nonlocal models are integro-differential equations (IDEs) and possess several modeling advantages over PDEs. The authors propose an inequality-constrained least squares approach that guarantees the well-posedness of the extracted models. The method provides additional utility including numerical homogenization as well as the ability to learn computationally cheap approximations of nonlocal operators of fractional-type while preserving accuracy. Several examples are presented in the paper, along with a discussion of open challenges in scaling these concepts to large-scale datasets and more complex applications [14].

Tajdari, Pawar, Li, Tajdari, Maqsood, Cleary, Saha, Zhang, Sarwark, and Liu [15] present a data-driven approach to predicting Adolescent Idiopathic Scoliosis (AIS) in their paper “Image-based modelling for Adolescent Idiopathic Scoliosis: Mechanistic machine learning analysis and prediction." The paper describes a technique for generating patient-specific geometric clinical data extracted from 2D X-ray images. A mechanistic machine-learned neural network is introduced, in which physics information governing nonuniform bone growth is incorporated into the data-driven model. This combined mechanistic/data-driven model is shown to more accurately predict the curve progression of the spine compared to a model based solely on clinical data. This powerful technique provides physicians with real-time information that can inform patient-specific treatment options [15].

The readers are referred to the following link to find the full papers of the special issue: https://www.sciencedirect.com/journal/computer-methods-in-applied-mechanics-and-engineering/special-issue/10W0KHX9CBQ

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