Guest Editorial

Special Issue: Scientific Machine Learning for Manufacturing Processes and Material Systems

Editorial Board consists of (alphabetically by last name)
Dr. Anindya Bhaduri, GE Research, USA, Anindya.Bhaduri@ge.com
Prof. Francisco Chinesta, ENSAM Institute of Technology, France, Francisco.CHINESTA@ensam.eu
Prof. Elias Cueto, University of Zaragoza, Spain, ecueto@unizar.es
Prof. Dehao Liu, Binghamton University, USA, dehaoliu@binghamton.edu
Dr. John G. Michopoulos, Naval Research Laboratory, USA, john.g.michopoulos.civ@us.navy.mil
Dr. Sandipp Krishnan Ravi, GE Research, USA, SandippKrishnan.Ravi@ge.com
Prof. Jian-Xun Wang, University of Notre Dame, USA, JWANG33@nd.edu

Computational modeling, simulation and optimization of manufacturing processes and materials systems have been a persistent endeavor of the engineering research community at large. Significant progress has been achieved in this field due to the exponential increase in computing power, and the incorporation of data-driven modeling methods. Process and systems modeling often involves expensive and time-intensive simulations and experiments. Incorporation of machine learning (ML) models as efficient surrogate models has been proven to enhance the human understanding on the behavior of the system at hand, and reduce the computational optimization cost of the concerned processes and systems. However, there is a rising need to go beyond the conventional data-driven techniques to address challenges, such as, presence of noise in data, limited budget, data sparsity, lack of interpretability of ML models, etc. Tackling these issues will enable more comprehensive modeling of manufacturing processes and discovery of novel material systems.

This special issue focuses in the new paradigm called scientific ML, and aims to explore and potentially resolve issues related to improving computational efficiency, incorporating domain-awareness, improving interpretability and robustness into the models and modeling techniques. In particular, this special issue has invited both full research and review papers focusing on research advances in the areas of scientific machine learning for manufacturing processes and material systems. The announced topics of interest included but were not limited to the following topics:
(1) Physics-informed ML for process/materials design and optimization.
(2) Physics-informed ML for diagnostics, prognostics and process control.
(3) Uncertainty quantification in modeling (including physics-informed ML, etc.).
(4) Leveraging high-throughput framework for modeling and optimization.
(5) Efficient modeling through adaptive and active learning algorithms.
(6) Explainable AI and causal inference augmented predictive modeling.
(7) Exploring state-of-the-art ML algorithms in modeling and optimization.
(8) Understanding of systems through knowledge representation and reasoning.
(9) Leveraging data-fusion and multi-fidelity techniques in modeling.

As result of this call, this issue features nine papers delving into various topics, including:

probabilistic printability maps for laser powder bed fusion via functional calibration and uncertainty propagation; unsupervised anomaly detection via nonlinear manifold learning; a physics-informed general convolutional network for the computational modeling of materials with damage; multi-fidelity physics-informed generative adversarial network for solving partial differential equations; stochastic defect localization for cooperative additive manufacturing using gaussian mixture maps; stress representations for tensor basis neural networks: alternative formulations to finger-rivlin-ericksen; machine-learning metacomputing for materials science data; physics-informed fully convolutional networks for forward prediction of temperature field and inverse estimation of thermal diffusivity and a global feature reused network for defect detection in steel images.

Summaries of each of the nine papers published in this special issue are provided below.

Article JCISE-23-1151 "Probabilistic Printability Maps for Laser Powder Bed Fusion via Functional Calibration and Uncertainty Propagation" by Wu, Whalen, Ma and Balachandran, describes the development of an efficient computational framework for process space exploration in laser powder bed fusion (LPBF) based additive manufacturing technology. This framework aims to find suitable processing conditions by characterizing the probability of encountering common build defects. A Bayesian approach is developed for inferring a functional relationship between LPBF processing conditions and the unobserved parameters of laser energy absorption and powder bed porosity. The relationship between processing conditions and inferred laser energy absorption is found to have good correspondence to the literature measurements of powder bed energy absorption using calorimetric methods. The Bayesian approach naturally enables uncertainty quantification and its utility is demonstrated by performing efficient forward propagation of uncertainties through the modified Eagar–Tsai model to obtain estimates of melt pool geometries, which are validated using out-of-sample experimental data from the literature. These melt pool predictions are then used to compute the probability of occurrence of keyhole and lack-of-fusion based defects using geometry-based criteria. This information is summarized in a probabilistic printability map. It is found that the probabilistic printability map can describe the keyhole and lack-of-fusion behavior in experimental data used for calibration, and is capable of generalizing to wider regions of processing space. This analysis is conducted for SS316L, IN718, IN625, and Ti6Al4V using melt pool measurement data retrieved from the literature.

Article JCISE-23-1278 "Unsupervised Anomaly Detection via Nonlinear Manifold Learning" by Yousefpour, Shishehbor, Foumani and Bostanabad focuses on the fact that data anomalies are can be thought as samples that significantly deviate from the rest of the data and their detection can play a major role in building machine learning models that can be reliably used in applications such as data-driven design and novelty detection. The majority of existing anomaly detection methods either are exclusively developed for (semi) supervised settings, or provide poor performance in unsupervised applications where there are no training data with labeled anomalous samples. To bridge this research gap, the authors introduce a robust, efficient, and interpretable methodology based on nonlinear manifold learning to detect anomalies in unsupervised settings. The essence of our approach is to learn a low-dimensional and interpretable latent representation (aka manifold) for all the data points such that normal samples are automatically clustered together and hence can be easily and robustly identified. This low-dimensional manifold is learned by designing a learning algorithm that leverages either a latent map Gaussian process (LMGP) or a

deep autoencoder (AE). It is found that the proposed LMGP-based approach, in particular, provides a probabilistic perspective on the learning task and is ideal for high-dimensional applications with scarce data. The superior performance of proposed approach is demonstrated over existing technologies via multiple analytic examples and real-world datasets.

Article JCISE-23-1295 "A Physics-Informed General Convolutional Network for the Computational Modeling of Materials with Damage" by Janssen, Haikal, DeCarlo, Hartnett and Kirby, focuses on the issue that the adoption of machine learning (ML) methods in computational mechanics has been hindered by the lack of availability of training datasets, limitations on the accuracy of out-of-sample predictions, and computational cost. This work presents a physics-informed ML approach and network architecture that addresses these challenges in the context of modeling the behavior of materials with damage. The proposed methodology is a novel physics-informed general convolutional network (PIGCN) framework that features (1) the fusion of a dense edge network with a convolutional neural network (CNN) for specifying and enforcing boundary conditions and geometry information, (2) a data augmentation approach for learning more information from a static dataset that significantly reduces the necessary data for training, and (3) the use of a CNN for physics-informed ML applications, which is not as well explored as graph networks in the current literature. The PIGCN framework is demonstrated for a simple two-dimensional, rectangular plate with a hole or elliptical defect in a linear-elastic material, but the approach is extensible to three dimensions and more complex problems. The results presented in this article show that the PIGCN framework improves physics-based loss convergence and predictive capability compared to ML-only (physics-uninformed) architectures. A key outcome of this research is the significant reduction in training data requirements compared to ML-only models, which could reduce a considerable hurdle to using data-driven models in materials engineering where material experimental data are often limited.

Article JCISE-23-1369 "Multi-Fidelity Physics-Informed Generative Adversarial Network for Solving Partial Differential Equations" by Taghizadeh, Nabian and Alemazkoor propose a new method for solving partial differential equations using multi-fidelity physics-informed generative adversarial networks. The proposed approach incorporates physics supervision into the adversarial optimization process to guide the learning of the generator and discriminator models. The generator has two components: one that approximates the low-fidelity response of the input and another that combines the input and low-fidelity response to generate an approximation of high-fidelity responses. The discriminator identifies whether the input–output pairs accord not only with the actual high-fidelity response distribution, but also with physics. The effectiveness of the proposed method is demonstrated through numerical examples and compared to existing methods.

Article JCISE-23-1386 "Stochastic Defect Localization for Cooperative Additive Manufacturing Using Gaussian Mixture Maps" by Rescsanski, Shah, Tang, and Imani, is addressing the issue on how cooperative Robotic Additive Manufacturing (RAM) suffers from the same defect generation challenges as conventional systems, thus necessitating improvements in the detection and prevention of flaws within fabricated components. Quality assurance can be further bolstered through the integration of AM models, which utilize sensor feedback to localize defects, vastly reducing false positives. This research explores defect localization through a novel dynamic defect model created from simulated sensing data. In particular, two cooperative robots are simulated to estimate defect parameters, while observing the workspace and accurately classifying different

regions of the part, generating a Gaussian mixture map that identifies and assigns appropriate actions based on defect types and characteristics. The experimental result shows that the implementation of the dynamic defect model and selective reevaluation achieved an effective defect detection accuracy of 99.9%, an improvement of 9.9% without localization. It has been shown that the proposed framework holds potential for application in domains that utilize high degrees-of-freedom machines and collaborative agents, offering scalability, improved fabrication speeds, and enhanced mechanical properties.

Article JCISE-23-1423 "Stress Representations for Tensor Basis Neural Networks: Alternative Formulations to Finger–Rivlin–Ericksen" by Fuhg, Bouklas and Jones, focuses on the fact that data-driven constitutive modeling frameworks based on neural networks and classical representation theorems have recently gained considerable attention due to their ability to easily incorporate constitutive constraints and their excellent generalization performance. In these models, the stress prediction follows from a linear combination of invariant-dependent coefficient functions and known tensor basis generators. However, thus far the formulations have been limited to stress representations based on the classical Finger–Rivlin–Ericksen form, while the performance of alternative representations has yet to be investigated. This work surveys a variety of tensor basis neural network models for modeling hyperelastic materials in a finite deformation context, including a number of so far unexplored formulations which use theoretically equivalent invariants and generators to Finger–Rivlin–Ericksen. Furthermore, potential-based and coefficient-based approaches are compared, as well as different calibration techniques. Nine variants are tested against both noisy and noiseless datasets for three different materials. Theoretical and practical insights into the performance of each formulation area also given.

Article JCISE-23-1439 "Machine-Learning Metacomputing for Materials Science Data" by Steuben, Geltmacher, Rodriguez, Birnbaum, Graber, Rawlings, Iliopoulos, and Michopoulos, addresses the issue that materials science data almost invariably require various post-acquisition computation efforts to remove noise, classify observations, fit parametric models, or perform other operations. Recently developed machine-learning (ML) algorithms have demonstrated great capability for performing many of these operations, and often produce higher quality output than traditional methods. However, it has been widely observed that such algorithms often suffer from issues such as limited generalizability and the tendency to "over fit" to the input data. In order to address such issues, this work introduces a metacomputing framework capable of systematically selecting, tuning, and training the best available machine-learning model in order to process an input dataset. In addition, a unique "cross-training" methodology is used to incorporate underlying physics or multiphysics relationships into the structure of the resultant ML model. This metacomputing approach is demonstrated on four example problems: repairing "gaps" in a multiphysics dataset, improving the output of electron back-scatter detection crystallographic measurements, removing spurious artifacts from X-ray microtomography data, and identifying material constitutive relationships from tensile test data. The performance of the metacomputing framework on these disparate problems is discussed, as are future plans for further deploying metacomputing technologies in the context of materials science and mechanical engineering.

Article JCISE-23-1469 "Physics-Informed Fully Convolutional Networks for Forward Prediction of Temperature Field and Inverse Estimation of Thermal Diffusivity" by Zhu, Zheng and Lu, address the issue that traditional Physics-informed neural networks (PINNs) suffer from low

accuracy and efficiency due to the fully-connected neural network framework and the method utilized to incorporate physical laws. In this paper, a novel physics-informed learning architecture, named physics-informed fully convolutional networks (PIFCNs), is developed to simultaneously solve forward and inverse problems of thermal conduction. The use of fully convolutional networks (FCNs) significantly reduces the density of connections leading to a computational cost reduction. With the advantage of the nodal-level match between inputs and outputs in FCNs, the output solution is be used directly to formulate discretized PDEs via a finite difference method, which is more accurate and efficient than the traditional approach in PINNs. The results demonstrate that PIFCNs can flexibly implement Dirichlet and Neumann boundary conditions to predict temperature distribution. Remarkably, PIFCNs can also estimate unknown thermal diffusivity with an accuracy exceeding 99%, even with incomplete boundaries and limited sampling data. It shown that the results obtained from PIFCNs outperform those obtained from PINNs.

Article JCISE-23-1577 “A Global Feature Reused Network for Defect Detection in Steel Images” by Yang, Wang, Liu and Cheng focuses on the topic of accurate detection of surface defects for steel that is essential to improve surface quality and service life. It has been shown that Deep learning (DL) used in steel surface defect detection can solve the problems of low efficiency and poor accuracy of traditional manual detection. The classic YOLOv5 as a DL method is used to accomplish defect detection tasks without attention mechanisms, resulting in a loss of global information. Besides, it is difficult to complete complex network detection tasks with low-configuration hardware, especially for surface defects with complex defect types and variable defect sizes. To address these issues, this paper introduces an improved global feature reuse and hardware-aware YOLOv5 by using BoTNet, RepGhost, and EfficientRep model (BGE-YOLOv5). The multi-head self-attention layer is used to obtain global information and only part of the convolutional layers is replaced to avoid the excessive computational cost. The RepGhost model is introduced to extract the remaining feature information for feature reuse. EfficientRep is used to replace the original structure to achieve hardware-aware and to balance the detection veracity and efficiency. The distance IOU is replaced by SCYLLA-IOU to accelerate the iteration and improve stability. The results of the framework on the surface defect database (NEU-DET) show that BGE-YOLOv5 achieves a mean average precision of 79.5%, which is 10.3% greater than the baseline. The proposed BGE-YOLOv5 has a better performance in steel surface defect detection.

In conclusion, this special issue features innovative approaches for adequate representation and techniques applicable to a diverse range of scientific ML applications in manufacturing processes and material systems in general. It is our hope that readers will find these papers insightful and thought-provoking, fostering further research in this field. The guest editors of this special issue extend their sincere gratitude to all the authors and reviewers for their remarkable contributions. Additionally, we acknowledge the unwavering support of Professor Yan Wang, the current Editor-in-Chief of JCISE. Our profound appreciation goes to Ms. Amy Suski for her timely reminders and administrative support.