

The 20<sup>th</sup> IEEE International Conference on Machine Learning and Applications  
(IEEE ICMLA-2021)

**Special Session: Machine Learning Surrogate Models in Science and Engineering**

December 13-16, 2021, Pasadena, California, USA

**Introduction**

Scientific observations, experiments, and simulations provide valuable data to train machine learning algorithms for constructing surrogate models, also known as metamodels, that assist in characterizing complex systems. The adoption of machine learning surrogate models holds the potential to significantly accelerate design space exploration and optimization when a closed analytical form that relates design parameters to performance criteria is unattainable. Examples of such systems abound in a wide range of scientific problems involving multiple scales, such as climate and power grid modeling, biological simulations, structural engineering, mechanics and materials, and integrated computational materials engineering. Hence, there is a growing interest to focus on the synergistic integration of traditional methods of scientific discovery and recent machine learning techniques, e.g., neural networks. Three fundamental research directions include: (1) assuring training data quality and adequacy under stringent resource constraints; (2) developing efficient, reliable, and physics-informed data-driven models to fully capture the behavior of complex systems; and (3) leveraging surrogate models for performing domain-specific tasks, such as optimization, sensitivity analysis, and uncertainty quantification.

**Scope**

This special session invites submissions of original works that address the above and other unique challenges of developing machine learning surrogate models in a broad range of science and engineering applications. Topics covered by this special session include but are not limited to:

- General methods for data acquisition, exploration, and analysis
- Active learning and optimal experimental design
- Feature extraction, selection, and dimensionality reduction
- Predictive modeling in the limited labeled data and/or weakly supervised case
- Machine learning methods for multimodal and heterogeneous data sources
- Scalability of machine learning algorithms
- Neural networks and probabilistic inference
- Physics-informed machine learning
- Developing surrogate models for complex systems and model evaluation
- Exploration and optimization of design spaces with machine learning surrogate models
- Multi-fidelity uncertainty quantification

## **Submission Guidelines and Instructions**

Submitted papers should conform to IEEE specifications with a maximum length of 8 pages. Manuscript templates can be downloaded from the [IEEE website](#). All submissions must be anonymized and may not contain any information with the intention or consequence of violating the double-blind reviewing policy, including (but not limited to) citing previous works of the authors or sharing links in a way that can infer any author's identity or institution, actions that reveal the identities of the authors to potential reviewers. Papers must be submitted via the [CMT System](#) by selecting the track "Special Session on Machine Learning Surrogate Models in Science and Engineering." Detailed instructions for submitting papers can be found on the [conference website](#).

## **Paper Publication**

Accepted papers will be published in the ICMLA 2021 conference proceedings (to be published by IEEE).

## **Important Dates**

Submission Deadline: **August 6, 2021**

Notification of Acceptance: **September 4, 2021**

Camera-ready Papers: **October 1, 2021**

Pre-registration: **October 1, 2021**

## **Special Session Organizers**

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