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Editorial

Artificial Intelligence in Modeling and Simulation

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1. Introduction

Modeling and simulation (M&S) serve as essential tools in various scientific and engineering domains, enabling the representation of complex systems and processes without the constraints of physical experimentation [1]. These tools have evolved significantly with the integration of artificial intelligence (AI), which offers advanced capabilities in essential aspects of M&S such as optimization [2,3], data analysis [4,5], and verification and validation [6]. AI's capacity to enhance M&S is demonstrated in applications ranging from engineering [7] and physics [8,9] to social sciences [10] and biology [11], providing novel approaches to problem-solving and system understanding.

In this Special Issue, entitled "Artificial Intelligence in Modeling and Simulation", we received 18 submissions from researchers worldwide. After a rigorous peer-review process, 11 papers were selected for publication, reflecting the diversity and depth of current research in the combined fields of AI and M&S. These papers encompass a wide range of topics, including the use of AI in developing and optimizing simulation models, AI-driven metamodeling, and the application of AI techniques in various domains such as industrial systems, agent-based modeling (ABM), and public health.

2. Contents

The accepted submissions can be broadly grouped into four main categories: (1) AI techniques for simulation and optimization [2,3], (2) AI in ABM [12], (3) AI for data processing and classification models [13], and (4) Artificial Neural Network (ANN) methods for improved M&S [14]. These are organized as follows:

AI techniques for simulation and optimization

1. Comparative Analysis of Classification Methods and Suitable Datasets for Protocol Recognition in Operational Technologies (2024), by Holasova et al., in *Algorithms* 17:208, https://doi.org/10.3390/a17050208.
2. A Biased-Randomized Discrete Event Algorithm to Improve the Productivity of Automated Storage and Retrieval Systems in the Steel Industry (2024), by Neroni et al., in *Algorithms* 17:46, https://doi.org/10.3390/a17010046.
3. Efficient Multi-Objective Simulation Metamodeling for Researchers (2024), by Ho et al., in *Algorithms* 17:41, https://doi.org/10.3390/a17010041.

AI in ABM

4. Exploring the Use of Artificial Intelligence in Agent-Based Modeling Applications: A Bibliometric Study (2024), by Ionescu et al., in *Algorithms* 17:21, https://doi.org/10.3390/a17010021.
5. A Largely Unsupervised Domain-Independent Qualitative Data Extraction Approach for Empirical Agent-Based Model Development (2023), by Paudel et al., in *Algorithms* 16:338, https://doi.org/10.3390/a16070338.
6. Validating and Testing an Agent-Based Model for the Spread of COVID-19 in Ireland (2022), by Hunter et al., in *Algorithms* 15:270, https://doi.org/10.3390/a15080270.

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Citation: Fachada, N.; David, N. Artificial Intelligence in Modeling and Simulation. *Algorithms* **2024**, *17*, 265. https://doi.org/10.3390/a17060265

Received: 11 June 2024
Accepted: 13 June 2024
Published: 15 June 2024

AI for data processing and classification models

7. Uncertainty in Visual Generative AI (2024), by Combs et al., in *Algorithms* 17:136, https://doi.org/10.3390/a17040136.
8. Framework Based on Simulation of Real-World Message Streams to Evaluate Classification Solutions (2024), by Hojas-Mazo et al., in *Algorithms* 17:47, https://doi.org/10.3390/a17010047.
9. CNN Based on Transfer Learning Models Using Data Augmentation and Transformation for Detection of Concrete Crack (2022), by Islam et al., in *Algorithms* 15:287, https://doi.org/10.3390/a15080287.

ANN methods for improved M&S

10. Comparing Activation Functions in Machine Learning for Finite Element Simulations in Thermomechanical Forming (2023), by Pantalé, in *Algorithms* 16:537, https://doi.org/10.3390/a16120537.
11. A Literature Review on Some Trends in Artificial Neural Networks for Modeling and Simulation with Time Series (2024), by Muñoz-Zavala et al., in *Algorithms* 17:76, https://doi.org/10.3390/a17020076.

These publications are described in detail in the following subsections, one per subject category.

2.1. AI Techniques for Simulation and Optimization

Several papers focus on the integration of AI techniques to enhance simulation and optimization processes.

In *Comparative Analysis of Classification Methods and Suitable Datasets for Protocol Recognition in Operational Technologies*, Holasova et al. analyze different machine learning methods for protocol recognition in operational technology (OT) networks, addressing the unique challenges of OT environments and highlighting the need for relevant datasets.

Neroni et al. present a hybrid approach in *A Biased-Randomized Discrete Event Algorithm to Improve the Productivity of Automated Storage and Retrieval Systems in the Steel Industry*, combining discrete event simulation with biased-randomized heuristics to minimize makespan in automated storage and retrieval systems, showcasing significant improvements over traditional methods.

In *Efficient Multi-Objective Simulation Metamodeling for Researchers*, Ho et al. introduce a methodology for multi-objective optimization using metamodels and heuristics, demonstrating the varying performance of different metamodel–optimizer pairs across several problem scenarios.

2.2. AI in Agent-Based Modeling

The application of AI within ABM is addressed in three studies featured in this Special Issue.

Ionescu et al. provide a bibliometric analysis in *Exploring the Use of Artificial Intelligence in Agent-Based Modeling Applications: A Bibliometric Study*, revealing trends and influential research in the convergence of these fields, with significant growth observed post 2006.

Paudel and Ligmann-Zielinska propose a novel approach in *A Largely Unsupervised Domain-Independent Qualitative Data Extraction Approach for Empirical Agent-Based Model Development*, using natural language processing tools to automate qualitative data extraction for ABM, reducing biases and improving efficiency.

Hunter and Kelleher detail the validation of an ABM in *Validating and Testing an Agent-Based Model for the Spread of COVID-19 in Ireland*, utilizing a scaling factor to manage computational costs while maintaining model accuracy in simulating pandemic dynamics.

2.3. AI for Data Processing and Classification Models

The potential of AI in improving data processing and classification models is demonstrated by three articles included in this Special Issue.

In the first of these articles, *Uncertainty in Visual Generative AI*, Combs et al. address the issue of uncertainty in generative AI models, proposing a pipeline to quantify uncertainty and improve model reliability.

In the following article, *Framework Based on Simulation of Real-World Message Streams to Evaluate Classification Solutions*, Hojas-Mazo et al. develop a simulation-based framework for enhancing the evaluation of message classification solutions under realistic conditions.

In the third article, *CNN Based on Transfer Learning Models Using Data Augmentation and Transformation for Detection of Concrete Crack*, Islam et al. focus on structural health monitoring in leveraging transfer learning and CNNs for accurate and efficient crack detection in concrete structures.

2.4. Artificial Neural Network Architectures and Methodologies for Improved Modeling and Simulation

ANNs are powerful tools for improving model efficiency and validity. The two final papers in this Special Issue address this theme, demonstrating the effectiveness of ANNs in complex simulation scenarios.

Pantalé investigates the impact of different activation functions on prediction accuracy and computational efficiency in *Comparing Activation Functions in Machine Learning for Finite Element (FE) Simulations in Thermomechanical Forming*.

Finally, Muñoz-Zavala et al. review trends in *A Literature Review on Some Trends in Artificial Neural Networks for Modeling and Simulation with Time Series*, summarizing ANN applications in time series prediction and suggesting future research directions.

3. Final Remarks

These papers highlight the substantial progress and varied uses of AI in modeling and simulation, offering useful insights and methods for both researchers and practitioners. The Editors thank all authors, reviewers, and the editorial team in making this Special Issue possible.

Author Contributions: Special Issue Editorial by N.F. and N.D. All authors have read and agreed to the published version of the manuscript.

Funding: This work was funded by Fundação para a Ciência e a Tecnologia under grants CEECINST/00002/2021/CP2788/CT0001 and UIDB/04111/2020.

Acknowledgments: The Editors would like to thank the authors of the submitted manuscripts and the reviewers for their contributions. The Editors would also like to thank the Managing Editor and supporting MDPI staff for their help in publishing this Special Issue.

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

Abbreviations

The following abbreviations are used in this manuscript:

ABM	Agent-Based Modeling
AI	Artificial Intelligence
ANN	Artificial Neural Network
FE	Finite Elements
M&S	Modeling and Simulation
OT	Operational Technology

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