

Emerging Computational Models for Scientific Discovery

Dr. Marjana Prifti Skënduli

Assistant Professor, University of New York Tirana (UNYT), Albania

Abstract

The rapid growth of computational capabilities has fundamentally transformed the process of scientific discovery by enabling researchers to analyse complex systems, process massive datasets, and develop predictive models beyond the limitations of traditional analytical approaches. Emerging computational models combine artificial intelligence, machine learning, high-performance computing, simulation techniques, and data-driven approaches to accelerate knowledge discovery across scientific disciplines. This research examines Emerging Computational Models for Scientific Discovery by analysing how advanced computational frameworks contribute to hypothesis generation, scientific modelling, predictive analysis, and interdisciplinary research innovation. The study adopts a conceptual research approach based on theoretical perspectives related to computational science, artificial intelligence, scientific modelling, data analytics, and digital research transformation. The analysis highlights that computational models enable researchers to explore complex phenomena through simulation, pattern recognition, automated reasoning, and intelligent prediction. Artificial intelligence-based models, deep learning systems, foundation models, and hybrid computational frameworks are creating new possibilities for scientific investigation in fields including physics, biology, chemistry, environmental science, and engineering.

The study identifies major challenges associated with emerging computational models, including computational resource requirements, model interpretability limitations, data quality issues, reproducibility concerns, ethical considerations, and the need for interdisciplinary expertise. Effective utilization requires transparent methodologies, responsible AI practices, and collaboration between computational scientists and domain experts. The research concludes that emerging computational models represent a significant transformation in scientific discovery by extending human analytical capabilities and enabling new forms of knowledge creation. Future scientific ecosystems will increasingly depend on intelligent computational frameworks that integrate automation, human expertise, and advanced modelling approaches.

Keywords: Computational Models, Scientific Discovery, Artificial Intelligence, Machine Learning, Scientific Computing, Data-Driven Research, Knowledge Discovery.

1. Introduction

Scientific discovery has historically depended on observation, experimentation, theoretical reasoning, and mathematical analysis. However, the increasing complexity of modern scientific problems has created new challenges that cannot always be addressed through conventional research approaches.

Complex systems such as climate dynamics, biological networks, material structures, and astronomical phenomena require advanced computational capabilities to analyse large-scale interactions and identify hidden patterns. Emerging computational models have become important tools for expanding scientific exploration by allowing researchers to simulate complex systems, process extensive datasets, and generate predictive insights. Computational science integrates mathematics, computer science, and domain-specific knowledge to create models capable of representing real-world phenomena through digital environments. These models provide researchers with opportunities to investigate processes that may be difficult, expensive, or impossible to study directly through physical experiments.

The development of artificial intelligence and machine learning has further transformed computational discovery approaches. AI-based models can analyse large volumes of scientific information, identify relationships within complex datasets, and support automated knowledge discovery. Modern computational approaches increasingly assist researchers in areas such as protein structure prediction, material discovery, climate modelling, and advanced engineering simulations. Scientific discovery is entering an era where computational models are becoming active components of research workflows rather than simple analytical tools. These systems can assist in generating hypotheses, evaluating possible explanations, and identifying promising research directions. Computational modelling of scientific discovery has developed as an important area within artificial intelligence research, focusing on how computational systems can contribute to scientific reasoning and knowledge generation.

High-performance computing has also played a significant role in enabling advanced scientific modelling. Large-scale computational resources allow researchers to perform simulations involving millions or billions of variables, creating opportunities for deeper understanding of complex scientific processes. The combination of high-performance computing, artificial intelligence, and large scientific datasets has created a new foundation for computationally enhanced discovery. Emerging foundation models and intelligent scientific systems are further changing the research landscape by supporting literature analysis, experimental planning, modelling assistance, and scientific reasoning. Recent developments suggest that AI-driven scientific systems are moving from supporting specific tasks toward broader frameworks capable of assisting multiple stages of scientific workflows.

Despite these advancements, computational models also create important challenges. Scientific researchers must address issues related to model transparency, reliability, computational cost, data limitations, and reproducibility. Complex AI models may generate accurate predictions while providing limited explanations regarding how conclusions are produced. The integration of computational models into scientific discovery therefore requires a balanced approach that combines technological innovation with scientific validation. Computational systems should enhance human scientific capabilities rather than replace critical reasoning and experimental verification.

2. Review of Literature

2.1 Evolution of Computational Science and Scientific Modelling

Computational science has developed from traditional mathematical modelling approaches into an interdisciplinary field combining computing technologies, simulation methods, and scientific theories. Early computational models primarily supported numerical calculations, whereas modern approaches enable complex simulations and predictive analysis.

Research indicates that computational modelling has become essential for understanding systems where direct experimentation is difficult or resource-intensive. These models support scientific investigation by representing physical, biological, and social processes within computational environments. The evolution of computational science reflects a shift from calculation-based approaches toward intelligent discovery systems capable of analysing patterns and generating scientific insights.

2.2 Artificial Intelligence and Machine Learning-Based Discovery Models

Artificial intelligence has introduced new possibilities for scientific discovery by enabling automated pattern recognition, prediction, and knowledge extraction. Machine learning models can process complex datasets and identify relationships that may remain difficult to detect through traditional analytical methods.

Deep learning approaches have been increasingly applied in scientific fields involving large and complex datasets. Research on deep learning for scientific discovery highlights opportunities in areas such as image analysis, sequential modelling, and graph-based scientific problems. AI-based discovery models provide significant advantages but require careful validation, transparency, and integration with scientific principles.

2.3 Data-Driven and Hybrid Computational Discovery Frameworks

Modern scientific discovery increasingly relies on data-driven and hybrid computational frameworks that combine simulations, machine learning, and domain expertise. These approaches allow researchers to integrate experimental data with computational predictions.

Hybrid models improve scientific understanding by combining the strengths of different analytical approaches. Computational simulations provide theoretical exploration, while AI methods enhance prediction and pattern discovery. Future scientific ecosystems are expected to increasingly depend on integrated computational frameworks that connect human researchers, artificial intelligence, and advanced scientific infrastructure.

3. Objectives of the Study

The primary objective of this study is to examine emerging computational models and analyse their role in transforming scientific discovery processes through advanced simulation, artificial intelligence, machine learning, and data-driven research approaches. The study focuses on understanding how computational frameworks improve scientific exploration, prediction capabilities, and knowledge generation across multiple disciplines.

The research further aims to explore the relationship between computational intelligence and scientific innovation by analysing how modern computational systems support researchers in identifying patterns, developing hypotheses, optimizing experiments, and interpreting complex scientific information.

The specific objectives of the study are:

- To analyse the conceptual foundations and major characteristics of emerging computational models used for scientific discovery.
- To examine the role of artificial intelligence, machine learning, high-performance computing, and simulation technologies in advancing scientific research.

- To explore how computational models support hypothesis generation, prediction, experimentation, and interdisciplinary scientific innovation.
- To identify technical, methodological, ethical, and reproducibility challenges associated with computational scientific discovery.
- To evaluate future directions for developing reliable, transparent, and intelligent computational frameworks for scientific advancement.

4. Research Methodology

4.1 Research Design and Conceptual Approach

This study adopts a conceptual research design based on qualitative analysis of existing academic literature, theoretical frameworks, and scholarly discussions related to computational science, artificial intelligence, scientific modelling, machine learning, and digital transformation of research practices. The conceptual approach is appropriate because the study aims to understand the broader influence of emerging computational models on scientific discovery rather than evaluate a particular computational system or experimental dataset. The research examines how computational approaches reshape scientific investigation by improving modelling capabilities, analytical efficiency, and knowledge generation.

The study integrates perspectives from computational science, artificial intelligence research, scientific methodology, information systems, and interdisciplinary innovation studies. Emerging computational models are conceptualized as intelligent research frameworks where algorithms, computational resources, scientific data, and human expertise interact to generate new scientific understanding. The research examines computational scientific discovery as a continuous process involving data acquisition, computational modelling, simulation, prediction, validation, interpretation, and knowledge dissemination. These stages demonstrate how computational approaches extend traditional scientific methods by providing additional analytical capabilities.

The study does not include primary experiments, laboratory validation, or statistical testing. Instead, it synthesizes existing theoretical knowledge to identify important computational approaches, scientific applications, implementation challenges, and future development opportunities. The methodology recognizes that computational models provide powerful analytical support but cannot independently replace scientific reasoning. Human researchers remain responsible for defining research questions, evaluating computational outcomes, and ensuring scientific validity.

4.2 Data Sources and Analytical Framework

The study utilizes secondary academic sources including peer-reviewed research articles, computational science publications, artificial intelligence studies, scientific modelling research, machine learning literature, and digital research transformation frameworks. A thematic analysis approach was applied to examine important dimensions including computational intelligence, scientific simulation, predictive modelling, data-driven discovery, model reliability, research reproducibility, and ethical considerations.

The analytical framework considers emerging computational models as integrated scientific ecosystems consisting of computational infrastructure, algorithms, scientific datasets, domain expertise, and discovery outcomes. The framework emphasizes that successful computational discovery requires alignment between technological capabilities and scientific objectives. Advanced computational systems

generate meaningful outcomes only when supported by reliable data, appropriate methodologies, and expert interpretation.

4.3 Conceptual Framework of Emerging Computational Models for Scientific Discovery

The proposed framework explains that computational scientific discovery develops through interconnected stages involving scientific data generation, computational processing, intelligent modelling, validation, and knowledge creation.The framework demonstrates how emerging computational approaches enhance traditional scientific methods by enabling deeper exploration of complex phenomena.

Table 1: Components of Computational Scientific Discovery Framework

Computational Component	Supporting Technology	Contribution to Scientific Discovery
Data Processing Systems	Big data analytics and scientific databases	Improved information management
Intelligent Modelling	Machine learning and deep learning	Pattern discovery and prediction
Simulation Frameworks	High-performance computing	Complex system exploration
Automated Analysis	AI-based reasoning systems	Faster scientific interpretation
Validation Mechanisms	Hybrid computational-experimental approaches	Improved reliability

5. Analysis

5.1 Artificial Intelligence-Based Models for Scientific Knowledge Discovery

Artificial intelligence has become one of the most influential computational approaches transforming modern scientific discovery. Traditional scientific methods often require extensive manual analysis, experimentation, and interpretation, whereas AI-based models provide capabilities for processing large datasets and identifying complex relationships. The analysis indicates that machine learning and deep learning models enable researchers to discover patterns within scientific information that may remain difficult to detect through conventional approaches. These models are increasingly applied in areas such as biological research, material science, astronomy, environmental modelling, and engineering systems.

AI-based computational models support scientific discovery by improving prediction accuracy and reducing the time required for analysing complex information. Researchers can use intelligent systems to identify potential relationships, evaluate possible outcomes, and prioritize promising research directions. In biological sciences, computational models assist researchers in understanding molecular structures, biological interactions, and complex genetic relationships. In physics and engineering, AI models support simulations and optimization processes involving highly complex systems.

The analysis further demonstrates that AI-based scientific models contribute to hypothesis development by identifying unusual patterns and suggesting possible research pathways. These capabilities transform computational systems from simple analytical tools into active components of scientific exploration. However, AI-generated insights require scientific verification. Computational predictions must be evaluated through theoretical reasoning, experimental validation, and domain expertise to ensure reliability. Therefore, artificial intelligence-based discovery models should be viewed as collaborative systems that enhance researcher capabilities while maintaining scientific oversight.

5.2 High-Performance Computing and Advanced Scientific Simulation

High-performance computing has become a fundamental component of modern computational science by enabling researchers to perform large-scale simulations and complex calculations. Many scientific problems involve enormous computational requirements that cannot be addressed through conventional computing resources. The analysis shows that high-performance computing allows researchers to model complex phenomena across various disciplines, including climate systems, astrophysical processes, molecular interactions, and advanced engineering applications.

Table 2: Applications of Computational Models in Scientific Fields

Scientific Field	Computational Application	Research Contribution
Physics	Numerical simulations	Understanding complex physical systems
Biology	Molecular and genomic modelling	Improved biological analysis
Chemistry	Computational chemistry models	Material and drug discovery
Climate Science	Environmental simulations	Future climate prediction
Engineering	Optimization models	Improved system design

Scientific simulation provides researchers with opportunities to explore scenarios that may be difficult to reproduce experimentally due to cost, time limitations, or safety concerns. Advanced computational models allow researchers to test theoretical assumptions, evaluate possible outcomes, and refine scientific understanding through repeated simulations.

The integration of artificial intelligence with high-performance computing further improves simulation capabilities by enabling faster analysis and adaptive modelling approaches. Nevertheless, computational simulations require accurate assumptions, reliable data, and appropriate validation methods. Incorrect model design or incomplete information can influence scientific conclusions.

5.3 Automated Hypothesis Generation and Intelligent Research Support Systems

Emerging computational models are increasingly supporting researchers in generating hypotheses and identifying new scientific possibilities. Traditional hypothesis development often depends heavily on human observation, theoretical reasoning, and existing knowledge structures. Intelligent computational

systems can analyse scientific literature, experimental data, and complex datasets to identify relationships that may suggest new research directions.

The analysis indicates that automated hypothesis generation can accelerate scientific discovery by reducing information-processing limitations and supporting interdisciplinary research. AI-based systems can connect knowledge from different scientific domains, enabling researchers to discover relationships that may not be obvious within specialized fields.

However, automated hypothesis generation requires careful evaluation because computational systems may identify statistical relationships without understanding deeper scientific meaning. Human researchers remain essential for evaluating the significance, feasibility, and theoretical relevance of computationally generated ideas. Future scientific research will increasingly involve collaboration between intelligent computational systems and human researchers to develop innovative discoveries.

6. Challenges

6.1 Computational Complexity and Resource Requirements

Emerging computational models often require significant computational resources, including advanced hardware, large-scale data storage, and specialized infrastructure. The increasing complexity of AI models and scientific simulations creates challenges related to energy consumption, computational costs, and accessibility. Research institutions with limited resources may face difficulties adopting advanced computational approaches. Developing efficient algorithms, shared research infrastructure, and collaborative computing environments is essential for expanding access to computational discovery tools.

6.2 Model Transparency and Scientific Interpretability

Many advanced computational models, particularly deep learning systems, operate as complex systems where decision-making processes are difficult to explain. Limited interpretability creates challenges for scientific researchers who require understanding of how computational predictions are generated. Transparent and explainable computational models are necessary to maintain scientific trust and reproducibility. Researchers must combine computational outputs with theoretical understanding and validation procedures.

6.3 Reproducibility, Data Quality, and Ethical Concerns

Scientific discovery depends on reliable and reproducible methods. Computational models may produce inconsistent results when datasets, algorithms, or computational environments differ. Data quality limitations can also influence computational outcomes and affect scientific reliability. Ethical considerations related to data usage, algorithmic bias, and responsible AI implementation require careful attention. Establishing transparent computational practices and responsible governance frameworks is essential for maintaining scientific integrity.

7. Discussion

7.1 Computational Models as Transformative Tools for Modern Scientific Discovery

The findings of this study demonstrate that emerging computational models have become transformative tools that are reshaping the process of scientific discovery. Traditional scientific approaches have

historically depended on observation, experimentation, and theoretical analysis; however, increasing complexity in scientific problems requires advanced computational capabilities capable of processing large-scale information and exploring complex relationships. The discussion highlights that computational models extend human scientific capabilities by enabling researchers to simulate complex systems, analyse extensive datasets, and generate predictive insights. These models provide additional approaches for understanding phenomena that may be difficult to investigate through conventional experimental methods.

Artificial intelligence-based computational systems have introduced new possibilities for scientific exploration by supporting pattern recognition, automated analysis, and knowledge discovery. Machine learning algorithms can identify relationships within scientific datasets and assist researchers in discovering meaningful patterns that may remain hidden through traditional analytical methods. Computational models have also strengthened interdisciplinary research by enabling collaboration between different scientific domains. Researchers from physics, biology, chemistry, environmental science, and engineering can utilize common computational frameworks to address complex problems requiring integrated knowledge. However, the discussion emphasizes that computational models should not be considered independent scientific decision-makers.

Scientific discovery requires theoretical understanding, experimental validation, and critical evaluation of computational outcomes. Human researchers remain responsible for interpreting results and establishing scientific significance. The effectiveness of computational discovery therefore depends on collaboration between intelligent systems and human expertise. Computational models provide analytical power, while researchers contribute creativity, scientific reasoning, and contextual understanding. Future scientific progress will increasingly depend on developing computational frameworks that enhance human discovery capabilities while maintaining scientific reliability, transparency, and ethical responsibility.

7.2 Integration of Artificial Intelligence and Scientific Knowledge Creation

The integration of artificial intelligence into scientific research has created new approaches for generating, organizing, and evaluating scientific knowledge. AI-supported computational models can analyse scientific literature, experimental data, and complex datasets to identify potential relationships and research opportunities. The discussion indicates that AI-based discovery systems are changing the role of computation within scientific workflows. Instead of being used only for calculations or simulations, computational systems are becoming active partners in knowledge exploration and research planning. AI models support scientific knowledge creation by accelerating information analysis and reducing the limitations associated with human processing capacity. Researchers can utilize intelligent systems to explore large research domains, identify emerging patterns, and develop new hypotheses.

The use of computational models is particularly valuable in areas where scientific data are highly complex or rapidly expanding. Fields such as genomics, climate science, astronomy, and materials research generate enormous datasets that require advanced computational methods for meaningful interpretation. Nevertheless, scientific knowledge creation through AI requires careful methodological consideration. Computational predictions must be evaluated through established scientific principles, experimental evidence, and theoretical consistency.

The discussion further emphasizes the importance of explainability and transparency in AI-driven scientific systems. Researchers must understand the basis of computational outcomes to ensure that discoveries are scientifically meaningful and reproducible. Future scientific ecosystems will increasingly combine artificial intelligence, computational modelling, and human expertise to create more efficient and innovative approaches to knowledge generation.

7.3 Future Directions for Intelligent Computational Discovery Ecosystems

The future of scientific discovery will increasingly depend on intelligent computational ecosystems that integrate artificial intelligence, high-performance computing, advanced simulation, and collaborative research platforms. These ecosystems are expected to provide researchers with more powerful tools for exploring complex scientific questions. One important future direction involves the development of autonomous scientific systems capable of assisting with multiple stages of research workflows, including data analysis, simulation design, hypothesis generation, and experimental planning. Advanced computational models may support personalized scientific assistance by adapting analytical approaches according to research objectives, available datasets, and disciplinary requirements.

The integration of quantum computing with computational science may further expand discovery capabilities by enabling new approaches for solving complex problems that exceed the limitations of traditional computing systems. Future computational ecosystems will also require stronger emphasis on open science, reproducibility, and responsible innovation. Transparent methodologies, accessible computational resources, and reliable validation mechanisms will be essential for maintaining scientific credibility.

International collaboration will become increasingly important as scientific discovery requires shared computational infrastructure, interdisciplinary expertise, and global knowledge exchange. The future of computational science will not depend only on technological advancement but also on developing responsible frameworks that ensure computational discoveries contribute positively to scientific progress and society.

8. Conclusion

Emerging Computational Models for Scientific Discovery represent a significant transformation in the evolution of scientific research. This study highlights that computational approaches have expanded scientific capabilities by enabling researchers to analyse complex systems, process large-scale datasets, and develop predictive models that support deeper understanding of natural and technological phenomena.

The analysis demonstrates that artificial intelligence, machine learning, high-performance computing, and advanced simulation frameworks are creating new opportunities for scientific exploration. These technologies support hypothesis development, knowledge discovery, predictive analysis, and interdisciplinary research collaboration.

Despite these advantages, computational scientific discovery involves important challenges related to computational requirements, model transparency, data quality, reproducibility, and ethical responsibility. Addressing these challenges requires strong methodological standards, responsible AI practices, and collaboration between computational experts and domain researchers.

The future of scientific discovery will increasingly involve intelligent computational systems that work alongside human researchers. Computational models can accelerate analysis and reveal hidden patterns, while human expertise remains essential for interpretation, validation, and scientific reasoning.

Emerging computational models should therefore be viewed as powerful scientific innovation frameworks that enhance rather than replace traditional research approaches. Through responsible development and integration, computational systems can contribute to faster, more reliable, and more comprehensive scientific discoveries.

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