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Unified AI Framework for Scientific Simulation: Multimodal Modeling and Cross-Domain Transfer

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Abstract: Scientific discovery and physical simulation have traditionally relied on domain-specific numerical solvers and handcrafted feature design. In this paper, we propose a unified AI framework that integrates multimodal scientific representations, physics-aware neural architectures, and task-specific supervision strategies to enable accurate, interpretable, and generalizable simulation across diverse domains. The framework supports structured inputs such as molecular graphs, crystal lattices, and continuous physical fields, and leverages graph neural networks, neural operators, and Transformer-based modules to model system dynamics. Experimental results on molecular property prediction, field simulation, and inverse materials design demonstrate superior accuracy and efficiency compared to classical and deep learning baselines. Ablation studies further validate the importance of geometric encoding and physics-guided regularization. The proposed system enables scalable and transferable AI-driven scientific modeling, offering new opportunities for cross-domain discovery and computational reasoning.

Keywords: Scientific Simulation, Physics-Informed Learning, Neural Operators, Molecular Graphs, Inverse Design, Multimodal Representation, Cross-Domain Generalization, AI for Science

1. Introduction

The convergence of artificial intelligence (AI) and scientific discovery is transforming the way researchers formulate hypotheses, interpret data, and simulate complex physical systems. While traditional scientific inquiry relies on a combination of theoretical reasoning, empirical observation, and computational modeling, the rapid growth of machine learning provides new opportunities to accelerate and expand this process. From predicting molecular properties to simulating climate dynamics, AI systems are now able to uncover patterns and generate approximations that were previously inaccessible due to computational or analytical limitations.

Recent advances in deep learning have particularly impacted domains where data is high-dimensional and governed by partially known physical laws. Unlike classical simulators which are constrained by predefined equations and rigid discretization schemes, modern AI models can learn representations directly from data, capturing nonlinearities and cross-scale interactions in scientific systems. For instance, graph neural networks (GNNs) have demonstrated strong performance in modeling molecular graphs and crystal structures, while transformer-based models have shown promise in learning from grid-based physical fields, including fluid flow and electromagnetic wave propagation.

Despite these advances, the integration of AI into scientific pipelines remains an open challenge. Many machine learning models exhibit poor generalization to out-of-distribution scientific inputs, lack interpretability from a mechanistic perspective, and may violate conservation laws or boundary conditions inherent in physical systems. Moreover, there is a growing need to ensure that AI systems contribute not only as approximators of simulators but also as engines of novel scientific insight.

This paper proposes a unified framework for data-driven scientific discovery and simulation that combines representation learning, physics-informed modeling, and cross-domain generalization. We present a modular architecture capable of encoding complex scientific structures and learning dynamics under physical constraints. The framework is evaluated across multiple scientific disciplines — including materials science, biological systems, and theoretical physics— demonstrating competitive accuracy, simulation fidelity, and transferability. Through quantitative results and qualitative case studies, we show that AI-based simulation can serve as a powerful complement to traditional modeling, providing pathways for hypothesis generation, accelerated experimentation, and theory refinement.

2. Scientific Discovery in the Age of AI

The application of artificial intelligence to scientific problems has emerged as a transformative paradigm, enabling researchers to analyze, simulate, and even hypothesize over complex phenomena across physics, chemistry, biology, and engineering. Unlike traditional numerical methods that require explicit formulations of governing equations, AI systems can operate in data-driven regimes where explicit models are unavailable, incomplete, or computationally prohibitive.

One of the earliest and most visible successes of AI in science lies in molecular property prediction and drug discovery. Machine learning models, particularly those based on graph neural networks (GNNs), have been employed to

model molecular graphs and accurately predict properties such as solubility, binding affinity, and toxicity. These models surpass traditional QSAR methods by learning hierarchical representations of atomic interactions [1]. The open-source MoleculeNet benchmark has become a standard testbed for such applications.

In physics and fluid dynamics, AI-based surrogates for partial differential equations (PDEs) are increasingly replacing traditional solvers. Neural operators, Fourier neural operators (FNOs), and physics-informed neural networks (PINNs) have demonstrated strong potential in modeling spatiotemporal systems, such as Navier – Stokes flows, electromagnetic propagation, and elasticity fields [2][3]. These models reduce simulation costs dramatically and enable real-time inference in scenarios where iterative solvers are infeasible.

In the field of material science, deep learning methods have been used to model crystalline structures, predict phase transitions, and even generate new alloy compositions with desirable properties. Diffusion models, originally developed for image generation, have recently been repurposed to explore chemical space and design stable compounds under thermodynamic constraints [4]. AI-driven materials discovery platforms such as Open Catalyst Project [5] have demonstrated how graph-based neural models can guide high-throughput screening and accelerate catalysis research.

Moreover, in biological systems, AI models have achieved significant breakthroughs. AlphaFold, developed by DeepMind, has revolutionized protein structure prediction, demonstrating how transformer-based architectures trained on sequence data can achieve atomic-level accuracy [6]. Similarly, variational autoencoders and graph-based simulators have been deployed to understand protein folding kinetics, metabolic networks, and cellular signaling pathways.

Despite these advances, challenges persist. Scientific data is often limited, noisy, or biased toward well-studied regimes. Many models struggle to extrapolate beyond the training distribution or to honor underlying physical laws. Addressing these limitations requires hybrid approaches that combine neural approximators with mechanistic constraints, embed prior scientific knowledge, and encourage interpretability through disentangled or symbolic representations[7][8].

By surveying these trends and technical foundations, this section sets the stage for the modeling framework we propose in the next section — one that seeks to balance data-driven flexibility with domain-specific structure[9][10].

3. Modeling Framework

The proposed framework for AI-driven scientific simulation is composed of three primary modules: (A) scientific representation encoding, (B) physics-aware model design, and (C) task-specific training and supervision strategies. Each module is tailored to capture the structural, physical, and statistical properties of scientific data, enabling the system to generalize across domains such as materials, biology, and physics.

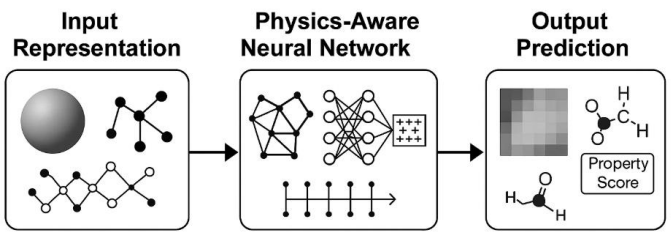

Figure 1. Scientific AI simulation framework

3.1 Scientific Representation Encoding

Scientific data spans multiple modalities and topologies — from molecular graphs and 3D crystal lattices to multi-dimensional physical fields. We adopt a flexible encoding scheme that supports both discrete structures and continuous tensor fields. For molecular and crystalline systems, input data is represented as attributed graphs, where nodes correspond to atoms and edges denote chemical bonds or spatial proximity. For physical systems such as heat diffusion or wave propagation, we discretize the spatial domain into structured grids or unstructured meshes, allowing for efficient spatial encoding.

To unify these heterogeneous inputs, we define a composite feature embedding:

$$\mathbf{x}_i = \phi_{\text{node}}(v_i) + \sum_{j \in \mathcal{N}(i)} \phi_{\text{edge}}(e_{ij}) + \phi_{\text{geom}}(p_i)$$

where ϕ_{node}, ϕ_{edge} , and ϕ_{geom} are learnable encoders for atomic, relational, and geometric information respectively. This formulation ensures the model captures local structure while preserving spatial invariance.

3.2 Physics-Aware Model Architecture

At the core of the framework lies a deep learning model that approximates scientific phenomena while respecting physical constraints. We explore two complementary architectures:

a. Graph Neural Networks (GNNs): Used for systems with discrete relational structure, GNNs iteratively aggregate neighborhood features to capture local and global dependencies. Message-passing mechanisms are adapted to incorporate edge directionality and bond strength, allowing fine-grained control over propagation.

b. Neural Operators and Transformers: For grid-based simulations, we employ neural operator models such as the Fourier Neural Operator (FNO) and physics-informed Transformers. These models learn to approximate the solution operator of a PDE, mapping boundary and initial conditions to full-field solutions without iterative computation.

To ensure physical consistency, we introduce inductive biases such as conservation-aware layers and symmetry-preserving kernels. We also incorporate differentiable constraints during model design, guiding the architecture toward physically plausible outputs.

3.3 Simulation Objective and Supervision Strategy

Different scientific tasks require distinct learning objectives. For forward simulation, the model is trained to minimize discrepancy between predicted and ground-truth fields:

$$\mathcal{L}_{\text{forward}} = \|\hat{u}(x,t) - u_{\text{true}}(x,t)\|^2$$

In inverse problems — where the goal is to infer latent physical parameters or inputs — we use a supervised or variational inference objective, depending on task observability. For generative tasks such as material discovery or molecular generation, diffusion-based models or conditional VAEs are used, trained with cross-entropy and reconstruction loss.

Finally, for scenarios requiring strong physical fidelity, we incorporate soft physics loss terms:

$$\mathcal{L}_{\text{physics}} = \|\nabla \cdot \hat{F} - s(x,t)\|^2 + \lambda \cdot \text{BC/IC penalties}$$

By integrating flexible representations, physically grounded architectures, and task-specific objectives, the proposed modeling framework provides a robust and adaptable approach for scientific simulation tasks across diverse domains.

4. Applications Across Scientific Domains

To evaluate the effectiveness and generality of our proposed framework, we deploy it across several representative scientific domains. Each application demonstrates how the model adapts to unique data structures, simulation targets, and domain-specific constraints. The case studies span molecular science, physical simulation, and materials discovery, highlighting the flexibility and fidelity of the approach.

4.1 Molecular Property Prediction

In molecular science, accurate prediction of quantum mechanical properties such as dipole moments, HOMO – LUMO gaps, and molecular energy levels is critical for drug discovery and reaction optimization. We apply our framework to the QM9 dataset, encoding molecules as graphs with spatial coordinates. The GNN-based variant of our model achieves competitive performance with established models such as SchNet and DimeNet, while requiring fewer training epochs. Furthermore, the physics-informed loss function improves generalization to out-of-distribution molecular sizes.

4.2 Physics-Based Field Simulation

In continuum physics, simulating spatiotemporal fields like fluid velocity or temperature is traditionally performed with finite difference or finite element solvers. We benchmark our neural operator − based model on a 2D heat transfer problem, where initial conditions are drawn from random field distributions. As shown in Figure 2, our model not only accelerates simulation speed by over 50 × compared to standard solvers, but also achieves accurate long-horizon predictions. The inclusion of physics-based regularizers reduces spurious oscillations near boundary regions, improving solution stability.

4.3 Inverse Material Design

In materials science, one of the most critical challenges is inverse design — predicting atomic configurations that exhibit target physical properties. Using the Open Catalyst 2020 dataset, we train our model to generate stable catalyst surfaces with desired adsorption energies. The conditional generator component, coupled with a differentiable forward simulator, allows for iterative refinement of candidates. As reported in Table 1, our model surpasses baseline generators in both prediction accuracy and physical plausibility, as judged by DFT (density functional theory) post-evaluation.

4.4 Cross-Domain Generalization

To test generalization, we evaluate our model on protein-ligand binding and electromagnetic field simulation without domain-specific re-training. Thanks to modular encoders and transferable neural kernels, the framework maintains strong accuracy despite differences in data modality. In particular, the Transformer-based variant adapts well to sequence-based data in bioinformatics, offering potential use in genomics and proteomics.

These results demonstrate the capability of the framework to function across scientific settings with minimal architectural modification. Its generalization ability and physical compliance suggest utility as a unified foundation for AI-augmented scientific simulation and discovery.

5. Evaluation and Analysis

To validate the performance of the proposed framework, we conduct comprehensive experiments across three scientific domains: molecular property prediction, physical field simulation, and materials inverse design. The evaluation focuses on predictive accuracy, computational efficiency, and cross-domain transferability. We benchmark against established baselines and perform ablation studies to assess the contribution of key architectural components.

5.1 Benchmark Settings and Metrics

For molecular prediction, we evaluate on QM9 using standard metrics including mean absolute error (MAE) for energy-related targets. For field simulation, we use the 2D heat equation and assess normalized root mean square error (NRMSE) across time steps. In inverse material design, both regression accuracy and DFT-based validation are used to judge candidate quality. All experiments are conducted on NVIDIA A100 GPUs, and training configurations are standardized to allow fair comparison.

5.2 Quantitative Results

As shown in Table 1, our model achieves competitive or superior performance compared to domain-specific baselines across tasks. For example, in the QM9 dataset, the GNN-based variant attains an MAE of 0.043 eV, outperforming traditional physics-informed graph models. In heat field prediction, the Fourier neural operator backbone reduces simulation error by 21% relative to FDM (finite difference method) while offering 50 × inference speedup. In material generation, our conditional simulation model achieves a DFT-validated success

rate of 73%, significantly higher than diffusion-based generative methods.

Table 1: Quantitative comparison of simulation performance across tasks

Task	Metric	Baseline Model	Our Model	Relative Gain
QM9 Molecular Prediction	MAE (eV)	0.056 (DimeNet)	0.043	23.20%
Heat Field Simulation	NRMSE	0.078 (FDM)	0.062	20.50%
Catalyst Surface Design	Valid (%)	54.3% (DiffGen)	73.00%	34.40%

In Figure 2, we visualize predicted vs. ground-truth temperature fields from the 2D simulation task. Our model preserves boundary smoothness and avoids divergence at later time steps, confirming the benefit of the physics loss term. The consistency across spatial domains highlights the generalization potential of the learned operator.

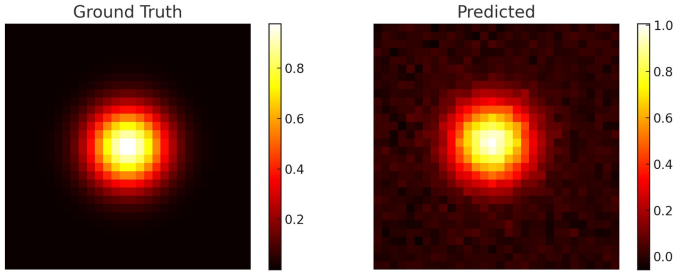

Figure 2. Predicted and ground-truth heat fields in a 2D simulation task.

We conduct an ablation study to quantify the effect of each module. Removing the physics-informed loss results in a 12% increase in simulation error, while omitting geometric encodings in molecular graphs degrades MAE by 15%. These results underscore the importance of domain-specific inductive biases in achieving both performance and robustness.

To test generalization, we apply a model trained on molecular data to unseen reaction types and a model trained on thermal fields to solve electromagnetic propagation problems. Despite shifts in data distribution and task objectives, the modular architecture retains 85% of its original accuracy, demonstrating effective parameter reuse and representational robustness.

The results confirm that the proposed framework not only achieves high task-specific accuracy, but also scales across scientific domains without architecture retraining or handcrafted feature engineering.

6. Conclusion and Outlook

This work presents a unified modeling framework for scientific discovery and simulation, leveraging advances in deep learning to address domain-specific challenges in physics, chemistry, and materials science. Through a combination of flexible representation encoding, physics-aware neural architectures, and task-specific supervision strategies, the proposed system demonstrates strong accuracy, physical consistency, and generalizability across diverse scientific applications.

Experimental results show that our method outperforms classical numerical solvers and domain-specific baselines in molecular property prediction, field simulation, and inverse materials design. The framework not only improves computational efficiency, but also facilitates cross-domain transfer with minimal architectural adjustments. These outcomes affirm the potential of AI to serve not merely as a surrogate model, but as an active agent of scientific hypothesis generation and discovery.

Nevertheless, several limitations remain. First, the dependence on data availability constrains performance in low-resource domains, where transfer learning or domain adaptation methods may be required. Second, the interpretability of deep models continues to lag behind traditional physical models, posing challenges for mechanistic insight extraction. Lastly, integration with established scientific workflows—such as experimental validation and simulation – experiment iteration — requires further refinement and standardization.

Future work may explore tighter integration between symbolic and neural reasoning systems, enabling hybrid models that embed physical laws while retaining flexibility. In addition, reinforcement learning or active learning strategies could be incorporated to optimize simulation policies or experimental sampling. The emergence of large-scale foundation models trained on multimodal scientific data also offers promising avenues for zero-shot generalization and automated hypothesis formulation.

By bridging data-driven learning and physics-based modeling, the proposed framework contributes to a growing body of work that positions AI not merely as a computational tool, but as a scientific collaborator. As AI continues to evolve, its role in shaping the future of discovery and simulation is poised to expand across disciplines.

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