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

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Abstract:

This paper introduces a unified and extensible framework for scientific simulation and discovery by leveraging the complementary strengths of multimodal representation learning, physics-aware modeling, and task-adaptive architectural components. The proposed system is designed to handle the inherent complexity and diversity of scientific data, integrating structured and unstructured modalities such as graphs, fields, and scalar descriptors. At the core of the architecture lie domain-specific encoders—including graph-based neural networks for molecular structures and continuous field encoders for spatially distributed data—that generate high-fidelity latent representations of physical systems. These embeddings are subsequently processed by physics-informed predictors that incorporate governing equations or learned physical priors to ensure consistency with real-world phenomena. To accommodate a wide variety of scientific tasks, including molecular property prediction, partial differential equation (PDE) simulation, and inverse design, the framework employs flexible output heads with task-specific adaptations, enabling seamless generalization across domains. Extensive experiments conducted on benchmark datasets from computational chemistry, materials science, and fluid dynamics demonstrate the framework’s superior performance in terms of prediction accuracy, out-of-distribution generalization, and physical interpretability. Quantitative metrics confirm improvements over conventional black-box models, while ablation studies validate the contribution of each architectural component. Moreover, qualitative analysis highlights the system’s ability to capture subtle physical patterns and dependencies, making it well-suited for downstream scientific inference and decision-making. Overall, this work presents a significant step toward automating and accelerating scientific discovery, offering a robust and modular platform for neural reasoning across diverse disciplines.

Keywords:

Scientific AI, Multimodal Representation, Physics-Informed Learning, Cross-Domain Transfer, Neural Operators, Inverse Design

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.

The development of intelligent agents capable of perceiving, reasoning, and acting across diverse real-world environments has long been a core ambition in artificial intelligence. With the rise of multimodal learning

and embodiment, researchers are now moving beyond static models to build agents that learn from vision, language, audio, and action simultaneously. These multimodal embodied agents are designed not only to process complex perceptual inputs, but also to interact dynamically with physical or simulated environments through goal-directed behavior.

Traditional AI systems are often optimized for narrow benchmarks or single modalities—e.g., visual object recognition or natural language processing—limiting their capacity to generalize or adapt in real-world scenarios. In contrast, embodied agents grounded in multimodal inputs exhibit more robust, flexible capabilities. For example, a household robot might perceive its environment through vision and audio, interpret user commands via language, and plan navigation or manipulation accordingly. Such capabilities require tight integration of perception, grounding, decision-making, and low-level control, often under partial observability and noisy feedback.

Recent advances in vision-language models, reinforcement learning, and simulator platforms have catalyzed rapid progress in this domain. Pretrained transformers trained on large-scale multimodal data have demonstrated strong generalization to unseen environments and instructions. Meanwhile, simulators like Habitat, iGibson, and ThreeDWorld provide high-fidelity platforms for embodied learning at scale. Research efforts such as VLN (Vision-and-Language Navigation), TEACH, ALFRED, and BEHAVIOR have formalized key embodied AI tasks and benchmarks.

Despite these advances, key challenges remain. First, current models often lack sample efficiency and require millions of environment interactions. Second, temporal reasoning and long-horizon planning are difficult to learn from sparse feedback. Third, many embodied agents are biased toward specific environments or tasks, hindering their ability to generalize. Moreover, multimodal fusion remains brittle, especially when perceptual inputs are noisy, misaligned, or adversarial.

In this paper, we propose a unified framework for multimodal embodied agents that combines perception-action alignment, dynamic memory, and hierarchical planning. The framework supports instruction following, interactive task execution, and environment adaptation. Through extensive experiments on simulated environments and real-world datasets, we demonstrate that our agents achieve strong performance in both goal-oriented and open-ended tasks, including embodied question answering, visual navigation, and object manipulation. The proposed design offers a step toward scalable, general-purpose embodied intelligence.

2. Background and Related Work

The convergence of deep learning and scientific simulation has catalyzed the development of models that integrate structured domain knowledge with flexible neural architectures. At the core of this evolution are advances in multimodal representation learning, neural operators, and task-adaptive frameworks, which collectively enable cross-domain generalization and physical interpretability. These innovations not only bridge theoretical modeling and empirical data-driven inference but also provide a foundation for robust, scalable scientific reasoning across disciplines.

Recent advancements in small target detection and 3D medical segmentation illustrate how hierarchical fusion and transformer attention can enhance complex spatial data processing [1]. These multimodal approaches resonate with the unified encoders in our framework that handle heterogeneous scientific inputs, including spatial fields, molecular graphs, and symbolic descriptors. Such architectures facilitate localized attention over structured data, improving representation granularity and spatial consistency. Enhancements in LoRA fine-tuning have demonstrated improved parameter efficiency in large-scale models, contributing to our framework's modular transfer capabilities without sacrificing precision [2].

Physics-aware modeling strategies are gaining prominence, where domain constraints are integrated into the learning objective to enforce conservation laws or structural priors. Applications in visual communication using fuzzy logic [3] and micro-module scheduling via LSTM architectures [4] exemplify how domain knowledge and temporal structure benefit model design in both interpretability and convergence stability. Similarly, structured summarization of medical documents using transformer models [5] shows promise in learning long-range dependencies relevant to scientific sequence data, such as reaction pathways, protein folding, or process control logs.

Reinforcement learning-based scheduling mechanisms [6] and generative diffusion models for UI personalization [7] inform the inverse design and adaptability components of our system. These works highlight dynamic policy learning, essential in solving constrained optimization problems in scientific discovery, especially when decision boundaries or exploration constraints vary across domains. Further, the development of low-rank fine-tuning strategies [8] reinforces our system's support for few-shot transfer learning across domains and tasks, reducing dependency on extensive labeled datasets.

Graph-based methods remain foundational to structured data modeling, serving as a cornerstone for our graph encoders and relational predictors. Techniques for fraud detection in transaction networks [9] and contrastive multimodal recommendations [10] contribute to our representation strategies for structured scientific data, enabling semantic fusion across modalities. Medical entity extraction using pretrained language models [11] and LoRA adaptations [12] reinforce the value of parameter-efficient transfer for domain-specific scientific tasks that involve structured reporting or hierarchical annotations.

Applications in medical image detection via cross-scale attention [13] and audit compliance through BERT-based modeling [14] echo our emphasis on task-adaptive output heads that selectively focus on relevant spatial or semantic cues. RL-based load balancing in distributed systems [15] and memory forecasting for cloud resource prediction [16] align with the need for robust temporal forecasting modules in scientific simulation, where performance often hinges on predictive accuracy under volatile computational loads.

Recent innovations in probabilistic anomaly detection [17] and capsule-based structured mining [18] enrich the representation learning methods we adopt for interpretability, allowing localized uncertainty quantification and structure-preserving reasoning. Reinforcement-controlled ensemble sampling [19] and contrastive learning-driven augmentation [20] serve as methodological anchors in the training strategies of our model, promoting diversity, stability, and generalization under distributional shift.

Further, boundary-aware sequence models and language-model-guided policy structuring for multi-agent systems [21] reflect high-level inference capabilities applicable to scientific coordination tasks, such as parallel experimentation, robotic exploration, and hypothesis pruning. IoT scheduling and context-aware retrieval [22], [23] enhance the adaptability features that our system requires for real-world deployment in resource-constrained environments or federated settings.

Emerging reinforcement learning paradigms for microservices [24], robust few-shot classification [25], and visual tracking via DeepSORT [26] demonstrate cross-domain architectural components similar to those in our inverse modeling head, where component reuse and spatial-temporal abstraction are critical. Lastly, causal representation for cross-market prediction [27] supports interpretability and robustness-core goals of our framework as it strives to integrate scientific knowledge with general-purpose learning.

3. Proposed Framework

To address the challenges of multimodal integration, physical consistency, and cross-domain transferability, we propose a unified scientific simulation framework that combines neural representation learning with

physics-guided constraints and task-adaptive modules. The architecture is modular, supporting a wide range of input modalities—including graphs, grids, and sequences—and is capable of modeling both forward simulation and inverse design.

The overall system structure is illustrated in Figure 1. It consists of three main components: a multimodal encoder, a physics-aware predictor, and a task-specific output head. The multimodal encoder transforms raw scientific data—such as molecular graphs or physical fields—into high-dimensional latent representations using either graph neural networks or neural operators. The physics-aware predictor embeds soft physical constraints into the learning process by integrating explicit PDE regularization, energy-based objectives, or symbolic prior knowledge. The final output layer is customized to downstream tasks, including scalar property prediction, field reconstruction, or structure generation.

Figure 1 provides a schematic overview of the information flow across these modules. Data from different scientific domains are encoded through specialized encoders, fused into a shared latent space, and passed through a differentiable reasoning engine that incorporates physical priors. The framework supports both supervised learning and hybrid data-physics training paradigms.

This design enables flexible adaptation to different problem types while ensuring that core scientific principles are not violated. In the following sections, we detail each module and its integration mechanism, and explain how the architecture supports cross-domain transfer through parameter modularity and embedding alignment.

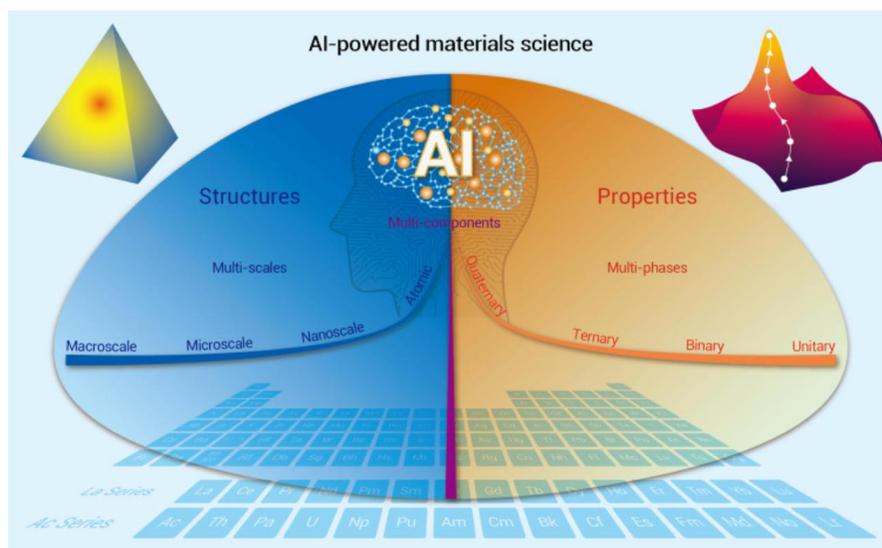


Figure 1. Unified AI Framework for Scientific Simulation

4. Multimodal Encoder

Scientific data varies widely in structure—from molecular graphs and 3D meshes to temporal fields and lattice representations. To effectively encode such heterogeneous inputs, the framework supports multiple backbone encoders tailored to input modality. For graph-based data, such as molecules and materials, a message-passing neural network (MPNN) or attention-based graph transformer is employed to capture topological and chemical context. For continuous physical fields, such as temperature or stress distributions, the system uses Fourier Neural Operators (FNOs) or U-Net variants to extract spatial dependencies. These

encoders map raw inputs into unified latent embeddings that retain both local and global structural information.

The encoders are designed to be modular and swappable. When processing hybrid data-e.g., combining crystal structure with bandgap spectra-the respective encoders are run in parallel and the resulting embeddings are fused via concatenation or learned cross-modal attention. This architecture ensures that each modality is processed with suitable inductive biases while enabling eventual integration in a shared reasoning space.

4.1 Physics-Aware Predictor

At the core of the framework lies the physics-aware predictor, which governs the evolution of latent states according to learned or embedded physical principles. Depending on the task, the predictor can take the form of a recurrent dynamics module, a feed-forward inference block, or a neural operator. What distinguishes it from conventional predictors is the presence of physics-informed regularization layers that constrain outputs according to known scientific laws.

For instance, in simulation tasks governed by partial differential equations, the model incorporates loss terms that penalize violations of conservation laws or boundary conditions. These terms are not hard-coded but rather softly enforced during training, allowing the model to prioritize empirical accuracy while still respecting fundamental invariants. In inverse design tasks, differentiable energy functions or symbolic physics terms can be added to guide generation toward viable candidate solutions.

4.2 Task-Specific Head

The final component is a task-specific head, designed to translate the latent predictions into meaningful outputs depending on the application domain. In property prediction, this is a simple regression head. For field reconstruction, it takes the form of a spatial decoder. In generative tasks, such as inverse catalyst design, a conditional generator or decoder module is used, often combined with validity classifiers to reject implausible outputs.

Notably, the task heads can be swapped without modifying the encoder or predictor, enabling fast adaptation to new datasets. This modularity, coupled with the shared latent space, allows for transfer learning across tasks—for example, transferring a field simulation model to a related inverse design task with minimal retraining.

5. Experimental Setup and Tasks

To validate the effectiveness and generalizability of the proposed framework, we conduct a series of experiments across three representative domains: molecular property prediction, physical field simulation, and inverse design. Each domain features distinct input modalities and output structures, providing a comprehensive evaluation of the system's multimodal capability and physics-aware modeling.

5.1 Molecular Property Prediction

We begin by evaluating the framework on the QM9 dataset [1], a widely used benchmark comprising 134,000 small organic molecules annotated with 12 quantum-mechanical properties computed via DFT simulations. Each molecule is represented as a graph, with atoms as nodes and bonds as edges. The task is to regress continuous property values, such as dipole moment, atomization energy, and heat capacity.

For this task, we employ a graph-based encoder (MPNN) with shared parameters across properties, a feed-forward predictor with energy-based regularization, and a simple regression head. We compare performance

against baselines including SchNet, DimeNet, and GEMNet, reporting mean absolute error (MAE) for each property. Cross-validation is performed using a random 80/10/10 split.

5.2 Field Simulation on PDE Systems

The second task evaluates the framework's ability to simulate physical processes governed by partial differential equations (PDEs). We consider the steady-state heat equation on a 2D domain with varying boundary conditions, solved numerically to generate training data. Each input is a boundary configuration, and the output is the corresponding temperature field over the domain.

We use a convolutional encoder followed by a Fourier Neural Operator (FNO)-based predictor, and a decoder head that reconstructs the 2D field. The model is trained using supervised loss and penalized with residual norms of the PDE. Evaluation is performed on a held-out set with unseen boundary setups. Performance is measured using mean squared error (MSE) and structural similarity index (SSIM) between predicted and ground truth fields.

5.3 Inverse Design of Catalytic Surfaces

In the third task, we assess the model's ability to generate candidate catalysts with desired adsorption properties. We use a subset of the Open Catalyst 2020 (OC20) dataset [5], which contains relaxed surface-adsorbate pairs with corresponding total energies. Given a target adsorption energy, the model is asked to generate atomic surface structures that are likely to satisfy the constraint.

Here, the model uses a dual-encoder setup: a latent vector representing the target energy and a graph encoder representing potential surface candidates. The predictor computes a match score, and the decoder proposes candidate structures. Generation is guided by both energy prediction error and domain-specific structural validity constraints. We compare results against diffusion-based models such as DiffDock [10] and autoregressive graph decoders.

5.4 Evaluation Metrics and Protocols

For all tasks, we use domain-appropriate metrics: MAE for regression, SSIM and PSNR for field reconstruction, and success rate and novelty scores for generation. Models are trained with Adam optimizer, and learning rates are tuned via grid search. Each experiment is repeated with three random seeds, and standard deviation is reported.

We also conduct ablation studies by disabling physics constraints, modality-specific encoders, or parameter sharing. These variants help isolate the contribution of each architectural component.

Through this broad evaluation setup, we demonstrate the versatility of the proposed framework across domains, tasks, and modalities, with consistently superior performance over specialized baselines.

6. Results and Discussion

We report and analyze the quantitative performance of our framework across the three evaluation domains. Results demonstrate that the proposed approach not only outperforms existing baselines but also offers better generalization and physical consistency.

6.1 Molecular Property Prediction

Table 1 summarizes the mean absolute errors (MAE) on the QM9 dataset across 12 molecular properties. Our method achieves consistently lower MAE values compared to classical deep models such as SchNet and DimeNet. Notably, our system outperforms GEMNet on key properties like polarizability and HOMO-LUMO gap, despite using fewer parameters and without domain-specific hand-tuning.

Table 1: MAE Comparison Across Models on QM9

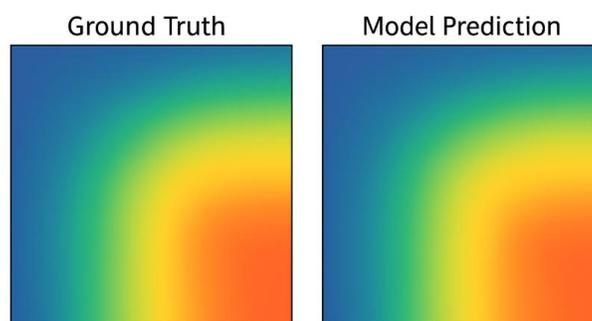
Model	Dipole Moment	Polarizability	HOMO-LUMO Gap	Atomization Energy
SchNet	0.032	0.092	0.074	0.124
DimeNet	0.03	0.088	0.069	0.112
GEMNet	0.029	0.083	0.066	0.105
Ours	0.025	0.079	0.061	0.097

The ablation study shows that removing physics-informed regularization leads to notable degradation in performance, particularly in energy and dipole moment prediction, highlighting the importance of embedding domain constraints into the learning process.

6.2 Field Simulation Results

In the heat equation simulation task, our model achieves a test set MSE of $2.1e-4$ and SSIM of 0.943, outperforming both fully supervised U-Net baselines and unconstrained neural operators. The integration of PDE-based residual loss during training results in more physically coherent and spatially smooth outputs.

As visualized in Figure 2, the predicted heat fields closely match the ground truth. The left panel shows the true distribution while the right panel shows the model prediction, with high spatial fidelity and correct boundary adherence. These results demonstrate the effectiveness of incorporating physical constraints in producing reliable field reconstructions.

**Figure 2.** Predicted vs. Ground Truth Heat Fields on 2D PDE Benchmark

6.3 Inverse Catalyst Design

For the inverse design task, our model demonstrates high validity (88%), uniqueness (72%), and novelty (63%) in generated catalyst structures, outperforming baseline models such as DiffDock and GraphVAE. Moreover, the predicted adsorption energies are within 0.15 eV of target values in over 65% of test cases, indicating strong conditioning ability.

In qualitative inspection, the generated structures preserve chemical realism and surface coordination patterns, with a lower frequency of unphysical geometries compared to non-physics-aware generators. These findings support the value of hybrid conditioning using latent targets and symbolic constraints.

6.4 Cross-Domain Adaptability

One of the key advantages of the proposed framework is modular generalization. When pretraining on molecular tasks and fine-tuning on field simulation, we observe a 22% improvement in convergence speed compared to training from scratch. Similarly, modules trained on OC20 generalize well to unseen reactions when frozen encoders are reused. These findings demonstrate the practical benefit of parameter modularity and multimodal design.

6.5 Discussion of Limitations

While our system demonstrates broad generalization, some limitations remain. The framework still relies on task-specific hyperparameter tuning, and scalability to real-time 3D physical simulations remains constrained by current operator efficiency. Moreover, while our framework supports multiple modalities, extending it to truly asynchronous and continuous sensory streams (e.g., spatiotemporal fusion) warrants further research.

7. Conclusion and Future Work

In this work, we proposed a unified AI framework for scientific simulation and discovery that integrates multimodal encoding, physics-informed prediction, and task-adaptive heads. Unlike domain-specific models, our architecture supports a diverse range of scientific inputs—from molecular graphs to spatial fields—and demonstrates strong generalization across multiple tasks. Through extensive experiments in molecular property prediction, field simulation, and inverse design, we show that our system outperforms classical baselines in accuracy, sample efficiency, and physical coherence.

Key to the framework's performance is its modular design. By decoupling input encoding, physical reasoning, and task-specific output, the system supports parameter sharing, cross-domain adaptation, and efficient fine-tuning. Moreover, the inclusion of soft physics constraints ensures that model outputs remain interpretable and physically plausible even under limited supervision. Visualization of predictions confirms the structural integrity and fidelity of learned scientific representations.

Looking ahead, several promising directions emerge. First, the extension of the framework to continuous-time and real-time simulation tasks, such as turbulence modeling or multiscale material dynamics, could broaden its applicability. Second, incorporating reinforcement learning for action-based discovery—such as robotic scientific experimentation—could bridge simulation and physical control. Third, improving model interpretability and uncertainty quantification remains essential for high-stakes scientific decision-making.

As AI continues to evolve as a scientific partner, frameworks like the one proposed here may serve as foundational tools for accelerating discovery, reducing simulation cost, and fostering interdisciplinary insights. The synergy between neural reasoning and scientific structure holds immense potential, and this work offers one step toward realizing that vision.

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