

AI as a Catalyst Across STEM: Engineering the Next Era of Discovery

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Abstract

Artificial intelligence (AI) has emerged as a critical set of computational methods and engineered systems that support discovery across science, technology, engineering, and mathematics (STEM) disciplines. While initially developed within computer science, AI applications are now widely utilized to achieve monumental advances across multiple domains, including:

1. **Biology and Medicine:** AI-based models have enabled real-time protein folding predictions that enhance drug discovery and precision healthcare.
2. **Climate Science:** Machine learning techniques have improved environmental modeling and long-term forecasting.
3. **Materials Engineering:** Computational algorithms have accelerated the design of alloys, polymers, and nanomaterials; and
4. **Astrophysics:** Large-scale data analysis methods support the interpretation of complex astronomical observations.

This paper examines the engineering foundations enabling AI-driven advancements. Relative emphasis was placed on the integral role of infrastructure, algorithm design, and governance frameworks in ensuring that AI applications remain scalable, ethical, and resilient. Current research indicates that AI-enabled engineering not only accelerates innovation but also redefines the competencies required for the future STEM workforce.

By addressing opportunities and challenges, including issues of data quality, bias, and regulatory oversight, this work positions AI's influence across STEM as a paradigm shift with far-reaching implications. The analysis highlights the importance of interdisciplinary collaboration among engineers, scientists, and educators in navigating the ethical and societal complexities of AI integration, ensuring that innovation is both responsible and sustainable.

Introduction

Artificial intelligence (AI) is recognized as a general-purpose technology with the capacity to influence discovery and innovation across science, technology, engineering, and mathematics (STEM) disciplines (Brynjolfsson & McAfee, 2019; DeSantis, 2024). Adoption of AI methods and systems has accelerated at an unprecedented pace. Since 2020, investments in AI for scientific and engineering applications have increased by billions of dollars (UNESCO, 2021). This rapid expansion underscores

the urgency of examining how AI is being engineered and integrated into STEM fields to address complex problems and enable new modes of inquiry.

Recent advances illustrate the breadth of AI's role in research and applied science. In biology and medicine, algorithmic models have sustained accurate protein folding predictions, contributing to advancements in drug discovery and precision health strategies (Jumper et al., 2021). In climate science, machine learning approaches have improved environmental modeling, enhancing forecasting capabilities and informing policy responses to climate change (Rolnick et al., 2022).

In the engineering and materials science domains, computational frameworks have rapidly accelerated the design of polymers, alloys, and nanomaterials, reducing the time and cost associated with experimental testing (Butler et al., 2018). Within astrophysics, large-scale data analysis techniques have enabled researchers to interpret increasingly complex astronomical datasets, expanding the scope of exploration and simulation (Ntampaka et al., 2019).

Given the scale and significance of these current developments powered by AI, a comprehensive analysis of AI's engineering foundations is crucial. This paper examines the infrastructure, algorithmic approaches, and governance frameworks that shape AI-enabled applications across the STEM fields.

The aim in the current body of work is to highlight how AI engineering is redefining discovery, identify the opportunities and challenges associated with its integration, and outline recommendations for future research to ensure responsible and sustainable innovation across disciplines.

Problem Statement

Global reliance on artificial intelligence (AI) for scientific and engineering discovery has expanded substantially. Former research has discovered more than 70% of research-intensive sectors have reported integrating AI-based methods into their workflows (Dernis et al., 2023). Despite these advances, challenges persist in establishing standardized engineering frameworks that ensure the scalability, reliability, and ethical application of AI across various disciplines.

The general problem is that, while AI has been widely adopted in STEM fields, the absence of consistent engineering integration practices has resulted in uneven outcomes related to transparency, accountability, and reproducibility (Floridi & Chiriatti, 2020). The specific problem is that the existing body of literature tends to evaluate AI within siloed domains such as computer science, healthcare, materials science, or climate modeling without adequately addressing the cross-disciplinary engineering foundations necessary to sustain responsible and resilient deployment (Heaven, 2021).

This gap in the literature highlights the need for an analysis that situates AI within an engineering context encompassing multiple STEM disciplines. Addressing this problem is crucial for aligning scientific discovery with governance standards, mitigating risks such as bias and data quality issues, and preparing the STEM workforce to engage responsibly with AI-enabled tools. This paper responds to that gap by exploring how AI engineering can act as a catalyst for interdisciplinary innovation while ensuring compliance with technical and ethical standards.

Significance of the Paper

The significance of this paper rests on its potential to align AI-enabled engineering practices with both discovery and governance. Former studies have demonstrated that AI methods improve prediction accuracy in areas such as drug discovery, climate forecasting, and astrophysics; however, inconsistent engineering and governance frameworks pose risks to reproducibility, transparency, and accountability (Haibe-Kains et al., 2020; Floridi & Chiriatti, 2020). By situating AI within an engineering context that emphasizes infrastructure, algorithms, and regulatory compliance, this paper contributes to closing the gap between the rapid scientific adoption of AI and the need for structured, ethical deployment across various disciplines.

The implications extend beyond research outcomes to the future of the STEM workforce. As AI methods are integrated into scientific practice, engineers, scientists, and educators will need new skills in algorithmic literacy, data governance, and compliance management (DeSantis, 2024). This paper highlights how the development of these competencies can strengthen responsible innovation while reducing risks of misuse, bias, and inequities in access. In doing so, it contributes to applied knowledge that can guide policy-makers, institutions, and organizations in aligning AI's transformative potential with broader societal goals.

Methodology

This study employed an integrative literature review to synthesize empirical and conceptual evidence on how artificial intelligence (AI) engineering contributes across STEM disciplines (science, technology, engineering, and mathematics). Application of integrative review is appropriate when the objective is to combine diverse study designs and theoretical contributions into a coherent account for practice and future research methodologies (Snyder, 2019). To enhance transparency and reproducibility, reporting followed PRISMA 2020 guidelines (identification, screening, eligibility, and inclusion) adapted for integrative synthesis (Page et al., 2021).

Search Strategy

A comprehensive search was executed across IEEE Xplore, ACM Digital Library, PubMed, and Scopus between January and August 2025. Core queries combined controlled vocabulary (where available) and free-text terms with Boolean and proximity operators. Primary strings included:

"AI in STEM" OR "artificial intelligence" AND (science OR engineering).

"AI engineering" OR "engineering foundations" AND (algorithms OR infrastructure OR governance).

"AI science discovery" OR "machine learning" AND (materials OR climate OR biology OR astrophysics).

"AI ethics" OR "responsible AI" AND (reproducibility OR transparency OR accountability).

Reference lists of included articles were hand-searched to identify additional relevant studies. Select grey literature from intergovernmental or standards bodies (e.g., methodological or governance reports) was considered when it presented systematic methods or datasets relevant to engineering integration. Literature lacking methodological rigor was excluded at full-text review (Page et al., 2021).

Inclusion And Exclusion Criteria

Inclusion

- Peer-reviewed journal articles, conference papers, and high-quality reviews published 2018-2025.
- English language primarily.
- Studies that:
 - (a) examine AI methods applied in STEM domains and (b) describe at least one engineering dimension (e.g., algorithmic design choices, data pipelines/infrastructure, reliability, security/governance, scalability).

Exclusion

- Editorials/op-eds without method sections.
- Domain pieces using AI without any engineering integration detail.
- Non-STEM applications
- Non-English that were not translated to English by a credible source.
- Items prior to 2018 (except when a seminal methodological source was needed for appraisal or reporting guidance, e.g., Kitchenham & Charters, 2007).

Screening And Selection

Records were de-duplicated, then screened by title/abstract against the criteria. Full-text review assessed methodological rigor, clarity of engineering contributions, and relevance to cross-disciplinary synthesis. A PRISMA-style flow captured counts at each stage (identification, screening, eligibility, inclusion) to support auditability (Page et al., 2021).

Quality Appraisal

Given the heterogeneity of designs, the Mixed Methods Appraisal Tool (MMAT) 2018 was used to appraise qualitative, quantitative, and mixed-methods studies on criteria such as clarity of research questions, appropriateness of methods, coherence between data and interpretations, and reporting of limitations (Hong et al., 2018). For software and engineering-focused evidence syntheses, appraisal also considered traceability of data pipelines, availability of code or model cards, and reproducibility indicators, drawing on software-engineering review guidance (Kitchenham & Charters, 2007).

Data Extraction

A structured template captured:

1. bibliographic metadata;
2. STEM domain;
3. AI method class (e.g., deep learning, probabilistic modeling);
4. engineering dimensions (algorithm design, infrastructure/compute architecture, data governance, testing/validation, reliability/resilience, security/compliance);
5. outcomes (e.g., predictive accuracy, discovery speed, materials/performance metrics, forecast skill);
6. reproducibility artifacts (datasets, code, documentation); and
7. stated limitations and ethical considerations.

Synthesis Approach

Findings were integrated via conceptual/thematic synthesis. First, codes were aggregated within domains (biology/medicine, climate/environment, materials/engineering, astrophysics). Second, cross-domain patterns were mapped to engineering concerns (e.g., data lineage and governance, algorithmic robustness, scalable infrastructure, documentation, and auditability). The synthesis highlights convergences and gaps that inform a cross-STEM engineering perspective and a forward research agenda (Snyder, 2019; Page et al., 2021).

Limitations

Potential constraints include:

- Publication and database bias.
- Rapid methodological evolution in AI that may outpace indexing.
- Variability in reporting engineering details across disciplines.

These risks were mitigated through multi-database searches, backward citation chasing, explicit eligibility rules, and standardized appraisal with MMAT (Hong et al., 2018).

Theories From the Literature

Two theories emerged from the literature, Socio-Technical Systems (STS) Theory and Innovation Diffusion Theory (IDT). Each offers complementary perspectives on how AI is engineered, integrated, and adopted across STEM disciplines. Combination of these theories offers a structured blueprint for analyzing the research problem of uneven AI engineering practices, reproducibility challenges, and adoption gaps.

Socio-Technical Systems (STS) Theory

STS theory was introduced by Trist and Emery (1960) to illustrate how organizational effectiveness arises when social and technical subsystems are jointly optimized. Later applications expanded into systems engineering and human-computer interactions (Baxter & Sommerville, 2011). Within STEM, STS highlights the interaction between people, processes, and engineered technologies.

Key concepts include joint optimization, which claims that technical subsystems (e.g., algorithms, data infrastructure, validation pipelines) must be co-designed with social subsystems (e.g., governance policies, workforce skills, organizational culture), and work system design, which emphasizes the need for human roles and responsibilities to adapt to technical architectures.

STS was adopted because AI across STEM delivers rapid results but often lacks reproducibility and governance due to poor integration of technical and organizational factors. This theory frames AI engineering as a systems problem, in which the quality of discovery, transparency, and accountability depend on aligning infrastructures within governance processes.

Innovation Diffusion Theory (IDT)

Everett Rogers (2003) developed Innovation Diffusion Theory to explain how innovations extend through populations over time. The theory has been applied widely in technology adoption, healthcare, and education (Greenhalgh et al., 2004).

IDT identifies five core concepts: relative advantage, compatibility, complexity, trialability, and observability that determine adoption rates. These constructs map directly onto AI in STEM:

- *Relative advantage* captures performance gains from AI-enabled workflows.
- *Compatibility* reflects integration with existing disciplinary norms.
- *Complexity* refers to technical barriers.
- *Trialability* aligns with pilot projects or sandboxing.
- *Observability* links to the transparency of results and benchmarks.

This theory illustrates why AI adoption across STEM has been uneven, despite its proven capabilities. While tools like AlphaFold gained rapid visibility, other AI models in climate science or materials engineering struggle to scale due to issues of complexity, interpretability, or compatibility with existing research practices. IDT provides a structured lens to examine the diffusion of AI engineering practices across domains, helping to identify where adoption is facilitated and where structural barriers persist.

Justification for Theoretical Selection

These theories were chosen over alternatives (e.g., change management or cognitive theories) because they directly address both integration and adoption, the dual pillars of the research problem.

STS clarifies how engineered infrastructures and governance structures must co-evolve with human and organizational factors, while IDT clarifies how those systems diffuse and achieve sustained adoption. Together, they help explain the complexities of reproducibility, accountability, and adoption that frame the problem of inconsistent AI engineering across STEM.

This combined theoretical framework provides the foundation for this body of work by linking the technical design of AI systems to their organizational uptake. This thereby aligning the study's aims to achieve scalable, ethical, and resilient AI that supports broader STEM innovation goals.

Literature Review

Biology & Medicine

Current research in biology and medicine illustrates the guarantees and limitations of AI in discovery pipelines. Jumper et al. (2021) presented AlphaFold, which gained unprecedented accuracy in protein structure prediction and marked a milestone for computational support in drug discovery.

Subsequent studies have highlighted the reduction in experimental bottlenecks and expanded proteome coverage achieved by these methods (Tunyasuvunakool et al., 2021), however, challenges remain in validation, clinical translation, and reproducibility (Zhavoronkov et al., 2020).

These findings frame reproducibility and governance as key problems in biomedical AI, aligning with this paper's aim to assess engineering practices that promote reliability, transparency, and sustained use across STEM.

Climate & Environmental Science

In climate science, AI has enhanced predictive accuracy and decision support. Rolnick et al. (2022) reviewed over 100 applications, including emissions modeling, biodiversity forecasting, and renewable energy optimization. This review highlighted incessant barriers, including fragmented datasets, a lack of interpretability, and governance gaps that hinder the adoption of AI models in policy contexts.

These studies demonstrate that although measurable improvements exist, standardized data curation, reproducible pipelines, and governance frameworks remain underdeveloped. This reflects the broader problem of a lack of cross-disciplinary engineering foundations for AI integration.

Materials Science & Engineering

In materials science, Butler et al. (2018) and Schmidt et al. (2019) surveyed the application of machine learning for property prediction and inverse design. These studies highlighted the accelerated discovery of polymers, alloys, and nanomaterials through computational models, framing AI as a means of expanding the chemical design space while reducing development costs.

Simultaneously, each body of work cautioned against laboriously depending on data quality, descriptor engineering, and the reproducibility of computational workflows. This work highlights the dual nature of the problem: rapid AI adoption has driven advances, but weak engineering practices limit reproducibility and generalizability. This insight directly supports the study's focus on aligning engineering methods with innovation.

Physics & Space

In astrophysics, researchers Ntampaka et al. (2019) demonstrated that machine learning can sustain classification, parameter estimation, and simulation surrogates for cosmological data, presenting value for large datasets, but with challenges in uncertainty quantification and validation.

The study framed the problem as one of integration, embedding AI into physics pipelines while preserving methodological rigor. This aligns with this paper's aims of the necessity of standardized engineering methods across STEM to ensure transparency, reproducibility, and adherence to disciplinary standards.

Challenges: Data Quality, Bias, Interpretability, and Governance

Multiple studies conclude that without strong attention to reproducibility and transparency, AI use in STEM will remain limited. Haibe-Kains et al. (2020) highlighted these deficits and called for standardized reporting of datasets, code, and evaluation methods.

Datasheets for Datasets (Gebru et al., 2021) and Model Cards (Mitchell et al., 2019) frameworks address these gaps, but adoption remains uneven. Rudin (2019) reported that opaque black-box models reduce accountability in high-stakes settings and recommended interpretable alternatives.

Collectively, this literature shows that engineering and governance foundations including datasets, pipelines, and interpretability tools, are inconsistently developed. Building on these findings, this study argues that AI in STEM must integrate infrastructure, algorithms, and governance to ensure reliable, ethical, and sustainable innovation.

Conclusions and Recommendations

This study examined AI engineering across STEM, discovering that while it has accelerated discovery in biology, climate science, materials engineering, and astrophysics, progress remains uneven due to fragmented data pipelines, weak governance, and inconsistent practices. Such findings align with precursory research identifying reproducibility and transparency as key barriers to sustainable adoption (Haibe-Kains et al., 2020; Gebru et al., 2021; Rudin, 2019).

Key Findings and Interpretations

AI is accelerating breakthroughs across STEM, from protein folding (Jumper et al., 2021) to climate modeling (Rolnick et al., 2022), with evident gains in speed and scope of discovery. However, scalability and reproducibility depend on strong engineering practices. Prior studies identify the lack of robust infrastructures and validation pipelines as a persistent limitation (Butler et al., 2018; Schmidt et al., 2019).

Governance frameworks also remain underdeveloped, with gaps in accountability, transparency, and bias mitigation hindering adoption (Haibe-Kains et al., 2020). Building AI literacy in algorithmic principles, data governance, and compliance has therefore become essential for the STEM workforce (DeSantis, 2024).

Finally, cross-disciplinary collaboration is imperative, as sustainable progress relies on teams of domain experts, engineers, and governance specialists co-designing systems (Rolnick et al., 2022).

Implications for Policy and Practice

For managers and practitioners

- Implement compliance-by-design workflows.
- Embed explainability into deployment decisions.
- Enforce transparent documentation standards.

Managers can use this information to guide resource allocation toward reproducibility safeguards, workforce training, and ethical oversight.

For organizations

- Invest in interdisciplinary R&D hubs and AI-skills pipelines, ensuring that domain experts and engineers collaborate within standardized governance frameworks.

Institutions can apply these findings by integrating documentation requirements (datasheets, model cards) into research funding and evaluation criteria.

For policymakers

- Develop regulations that incentivize transparency and reproducibility while supporting innovation.

Policies that encourage the publication of open benchmarks and reproducible datasets can help standardize practice across disciplines.

Strengths and Limitations

The strength of this study lies in synthesizing findings across multiple STEM domains, showing that the problems of reproducibility, governance, and adoption are not isolated but systemic. The limitation is that much of the evidence is drawn from recent but rapidly evolving literature, which means that frameworks may require continuous updating as methods advance.

Perspectives for Future Work

Future research should

- Expand longitudinal studies that evaluate AI integration over time across disciplines.
- Develop cross-domain engineering frameworks that unify best practices in data governance, reproducibility, and lifecycle documentation.
- Explore policy implications through interdisciplinary collaborations between researchers, practitioners, and regulators.
- Examine workforce development strategies that prepare future STEM professionals to engage with AI responsibly.

Final Reflections

This study shows that AI's role in STEM is defined less by faster algorithms or larger datasets than by the engineering practices, governance frameworks, and collaborative infrastructures that sustain innovation.

The stakes extend beyond disciplinary advances: responsible integration of AI will determine whether discoveries are reproducible, ethical, and socially beneficial. Building on prior research and broader debates on governance and adoption, this paper not only diagnoses current challenges but also calls on researchers, managers, organizations, and policymakers to embed resilience and accountability into the future of AI in STEM.

Recommendations for Future Research

Building on the findings across biology and medicine, climate and environmental science, materials science and engineering, and astrophysics, this section outlines a forward agenda that addresses identified gaps in engineering practice, governance, and adoption. The goal is to guide researchers and organizations toward approaches that enhance reproducibility, accountability, and sustained impact across the STEM fields.

Identifying Research Gaps

- Cross-domain engineering standards.* Prior work demonstrates advances within individual domains but lacks shared engineering frameworks for data lineage, validation, uncertainty reporting, and documentation that travel across STEM domains (Haibe-Kains et al., 2020; Mitchell et al., 2019; Gebru et al., 2021).
- Evaluation under distribution shift.* Many studies report performance on static test sets; fewer examine out-of-distribution robustness or degraded conditions typical of real deployments (Koh et al., 2021; Abdar et al., 2021).
- Lifecycle governance.* Evidence of systematic, end-to-end auditing and post-deployment monitoring remains limited relative to need (Raji et al., 2020; Haibe-Kains et al., 2020).

Building on Current Findings

- Domain-informed, engineering-ready pipelines.* Extend successful exemplars—e.g., protein structure prediction (Jumper et al., 2021; Tunyasuvunakool et al., 2021), climate decision aids (Rolnick et al., 2022), materials inverse design (Butler et al., 2018; Schmidt et al., 2019), and cosmology workflows (Ntampaka et al., 2019)—by codifying pipeline patterns (data curation → model

development → validation → documentation → release) that can be adapted across disciplines.

- b. *Benchmarking regimes.* Create shared, versioned benchmarks with clear provenance, uncertainty targets, and governance artifacts (datasheets, model cards) to align reporting across communities (Mitchell et al., 2019; Gebru et al., 2021).

Methodological Improvements

- a. *Uncertainty quantification and calibration.* Incorporate calibrated confidence measures, coverage guarantees, and stress tests for critical use cases (Abdar et al., 2021).
- b. *Robustness to shift.* Evaluate methods on real-world distribution shifts using standardized suites (e.g., WILDS) and publish protocols for stress testing (Koh et al., 2021).
- c. *Reproducibility by design.* Require versioned datasets, computational environments, and executable pipelines; pair publications with code, data, and documentation to support independent verification (Haibe-Kains et al., 2020; Mitchell et al., 2019).
- d. *Human-AI workflow studies.* Examine interaction patterns, escalation protocols, and feedback loops that improve reliability and user trust in scientific settings (Amershi et al., 2019).

Exploring Alternative Perspectives

- a. *Complementary theoretical lenses.* Alongside the Socio-Technical Systems and Innovation Diffusion perspectives used here, future work can test Value Sensitive Design and related approaches to ensure that stakeholder values and institutional constraints are elicited and integrated into engineering choices (Friedman & Hendry, 2019).
- b. *Policy and economics interfaces.* Extend analyses to quantify how regulatory requirements, incentives, and funding models shape engineering decisions and diffusion across STEM (Dernis et al., 2023).

Cross-disciplinary Research

- a. *Consortia and living labs.* Establish multi-institution collaborations that operate shared data trusts, reproducibility centers, and governance boards spanning biomedicine, climate, materials, and astrophysics. These environments can accelerate translation by aligning engineering practices and compliance expectations across domains (Rolnick et al., 2022; Ntampaka et al., 2019).
- b. *Transferable infrastructure.* Develop modular reference architectures (ingestion, lineage, privacy, compute orchestration, monitoring) deployed across labs to evaluate portability and maintainability in heterogeneous settings.

Addressing Limitations

- a. *Broader evidence bases.* Expand beyond English-language and high-resource contexts; include negative results and replication studies to mitigate publication bias (Haibe-Kains et al., 2020).
- b. *Richer outcomes.* Complement accuracy metrics with cost, time-to-insight, safety, and equity indicators to align engineering with real-world constraints.

Extended timeframes and longitudinal studies

- a. *Post-deployment monitoring.* Conduct multi-year audits of AI-enabled pipelines in laboratories, observatories, and field programs to track model drift, error modes, and governance compliance (Raji et al., 2020).
- b. *Workforce development trajectories.* Study how training in data governance, interpretability, and compliance affects adoption and outcomes across teams over time (DeSantis, 2024).

Applications in Varied Contexts and Policy Implications

- a. *Contextual validation.* Test methods in diverse institutional settings—academic labs, public research institutes, and industry R&D—to understand transfer barriers.

- b. *Policy-aligned reporting*. Align documentation and uncertainty reporting with policy decision thresholds in health, climate, and infrastructure planning to support actionable, accountable use (Mitchell et al., 2019; Gebru et al., 2021).

These recommendations restate the central finding that engineering practice and governance determine whether AI advances scale responsibly across STEM into a concrete roadmap. By prioritizing standardized documentation, robust evaluation under shift, longitudinal monitoring, and cross-disciplinary infrastructure, future research can close gaps identified in prior work and enable reproducible, ethical, and durable innovation.

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