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Artificial Intelligence: Scientific Research's Powerful Paradigm

Muhammad Fahad Shinwari [1,*], Muhamad Zahim bin Sujod [1], Norhafidzah binti Mohd Saad [1], Sheeraz Iqbal [2], Junaid Ali [3] and Islam Ahmed [1]

[1] *Faculty of Electrical and Electronics Engineering, UMPSA, Pekan, Pahang, Malaysia.*
[2] *King Fahad University of Petroleum and Minerals, Dhahran, Saudi Arabia*
[3] *Faculty of Chemical and Process Engineering Technology, UMPSA, Gambang, Pahang, Malaysia*

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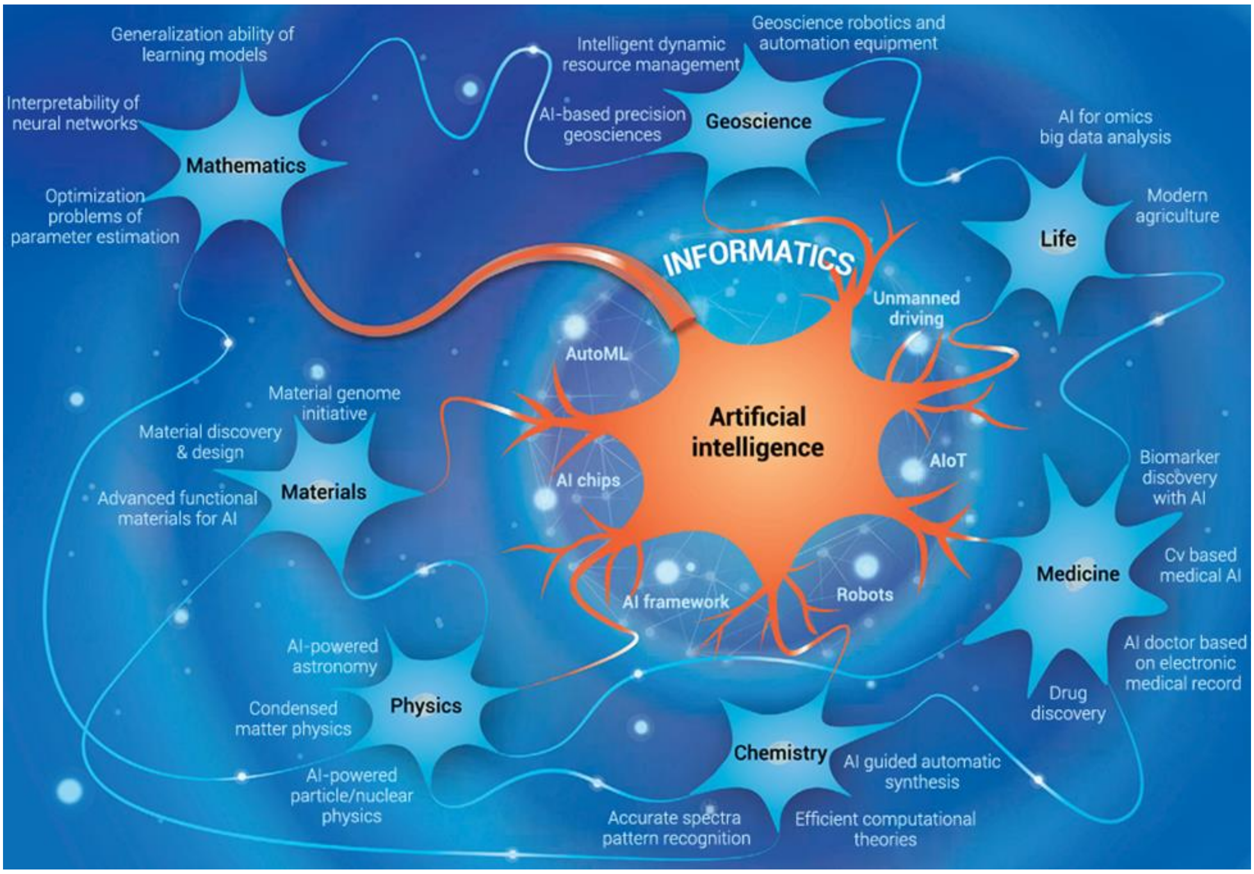
Abstract

Artificial intelligence (AI), together with modern machine learning (ML) and deep learning (DL), is reshaping research and practice across science, engineering, business, and everyday life. As scientific instruments and simulations generate increasingly large, high-throughput datasets, ML methods have become essential for extracting patterns, organizing information, forecasting outcomes, and supporting evidence-based decisions. This rewritten overview surveys how AI is being developed and applied across foundational disciplines, including information science, mathematics, medical science, materials science, geoscience, life sciences, physics, and chemistry. For each area, it highlights major bottlenecks (such as data scarcity, noisy observations, complex dynamics, and expensive experimentation) and explains how AI tools can help address them. It also outlines emerging research directions that deepen the integration of AI into scientific workflows. The goal is to provide a broad, readable guide to where AI can accelerate fundamental research and what practical challenges still need attention.

Keywords: Artificial intelligence; machine learning; Deep learning; Information science; Mathematics; Medical science; Materials science; Geoscience; Life science; Physics; Chemistry

* Corresponding author: Muhammad Fahad Shinwari

Graphical Abstract



1. Introduction

In 1950, Alan Turing famously asked whether machines could think. Rather than arguing over a strict definition of “thinking,” he proposed a practical test now known as the Turing test to evaluate whether a machine’s behavior could be indistinguishable from a human’s in conversation. In today’s language, AI refers to systems designed to emulate aspects of human intelligence, including perception, learning, reasoning, planning, and decision-making.

AI research spans many subfields, such as search and optimization, knowledge representation (including knowledge graphs), natural language processing, expert systems, evolutionary computation, and, most prominently in recent years ML and DL (Paul et al., 2020; Ullah et al., 2025). In parallel with waves of industrial automation, the next frontier is the automation of cognitive tasks that previously required human judgment.

A common way to describe AI capabilities is in three layers. First, perceptual intelligence enables machines to sense the world (vision, speech, touch). Second, cognitive intelligence supports abstraction, inference, and knowledge acquisition. Third, decision intelligence focuses on choosing actions, often under uncertainty to achieve goals. Making these layers work in practice requires a robust “infrastructure layer”: data pipelines, storage, compute, ML algorithms, and software frameworks. Together, these ingredients allow models to learn from data and power real-world applications that increasingly intersect with fundamental science, manufacturing, governance, and cyberspace.

Highlights

- AI seeks to build machines that can approximate human capabilities such as learning, reasoning, perception, prediction, and planning.
- When paired with ML/DL, AI is increasingly influential in core sciences from mathematics and physics to medicine, materials, and Earth systems.
- Rapid progress is enabled by an ecosystem of data resources, storage, compute, algorithms, and software frameworks that make AI easier to deploy.

2. A Brief History of Artificial Intelligence

Modern AI is often dated to 1956, when John McCarthy used the phrase “artificial intelligence” for a Dartmouth workshop, helping define the field. Early successes, especially in symbolic reasoning, fueled optimism. Researchers built programs that could prove mathematical statements or solve constrained algebraic problems. One emblematic system, Logic Theorist (Newell, Simon, and Shaw), demonstrated that computers could discover proofs and sometimes generate cleaner derivations than hand-crafted ones.

However, these early methods struggled with messy, real-world complexity. Many problems were too difficult for purely logic-driven programs, and computing resources were limited. As a result, funding and interest declined—an episode often called an “AI winter.”

AI regained momentum in the 1980s through expert systems, which encoded human expertise as collections of rules to support specialized decision-making. Systems such as XCON (Carnegie Mellon University) and MYCIN (Stanford University) showed that knowledge-based tools could be useful. Yet they also exposed drawbacks: expensive upkeep, limited flexibility, narrow scope, and practical concerns around deployment and privacy. When large national initiatives (such as Japan’s Fifth Generation project) failed to meet lofty expectations, support again diminished.

A major turning point arrived in the mid-2000s. Advances in training deep neural networks along with techniques that mitigated optimization issues such as vanishing gradients reinvigorated DL research (Bu et al., 2025; Shahzad et al., 2025; Ullah et al., 2025). At the same time, larger datasets and faster hardware (notably GPUs) made it feasible to learn representations directly from data. In many tasks in computer vision and natural language processing, DL systems began to match or surpass human performance on benchmark datasets. More broadly, ML became a powerful approach across data-intensive sciences because training a model from examples is often simpler than hand-coding rules for every situation.

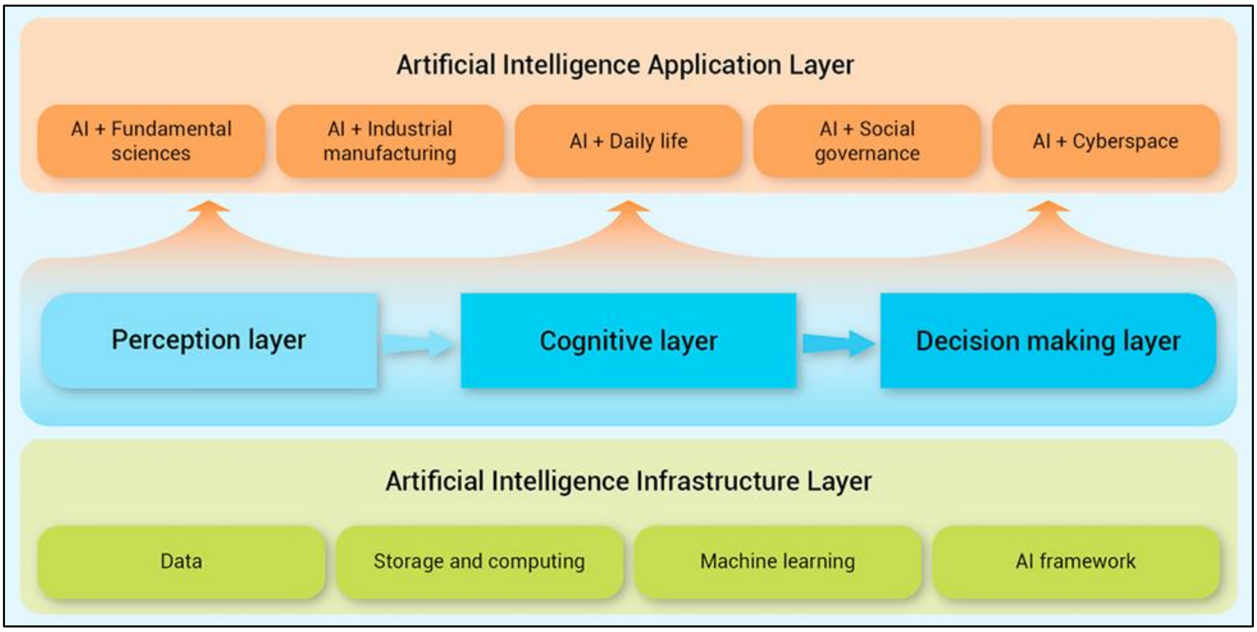


Figure 1 The General framework of AI

2.1. AI in Information Science

The information sciences both develop AI and benefit from it. Progress has accelerated because researchers can now rely on a mature AI stack that includes large datasets, scalable storage, high-performance computing, robust ML algorithms, and well-engineered software frameworks (Xu et al., 2021). These tools support applications across perception (e.g., computer vision and speech), cognition (e.g., language understanding, knowledge graphs, and continual learning), and decision-making (e.g., planning, expert systems, and decision support).

2.2. AI frameworks and platforms

Deep learning frameworks make it easier to build, train, and deploy neural networks by providing efficient tensor operations, automatic differentiation, GPU acceleration, and reusable model components (Alawi, 2025). Earlier tools such as MATLAB, OpenNN, and Torch were not built specifically for large-scale DL, and often required substantial expertise to use effectively. First-generation DL frameworks (e.g., Caffe, Chainer, and Theano) reduced friction and made common architectures CNNs, RNNs, and LSTMs more accessible (Hammad, Rahamaddulla, Sorooshian, et al., 2025; Paszke et al., 2019).

Major technology companies later expanded the ecosystem: TensorFlow (Google), PyTorch (originating from Facebook's AI research and Torch), CNTK (Microsoft), and MXNet (announced by Amazon). Frameworks differ in style: graph-based approaches can enable aggressive optimization, while eager/imperative execution is often simpler to debug and more flexible. Over time, platforms have improved APIs, distributed training support, multi-GPU scaling, and curated "model zoos" and toolkits.

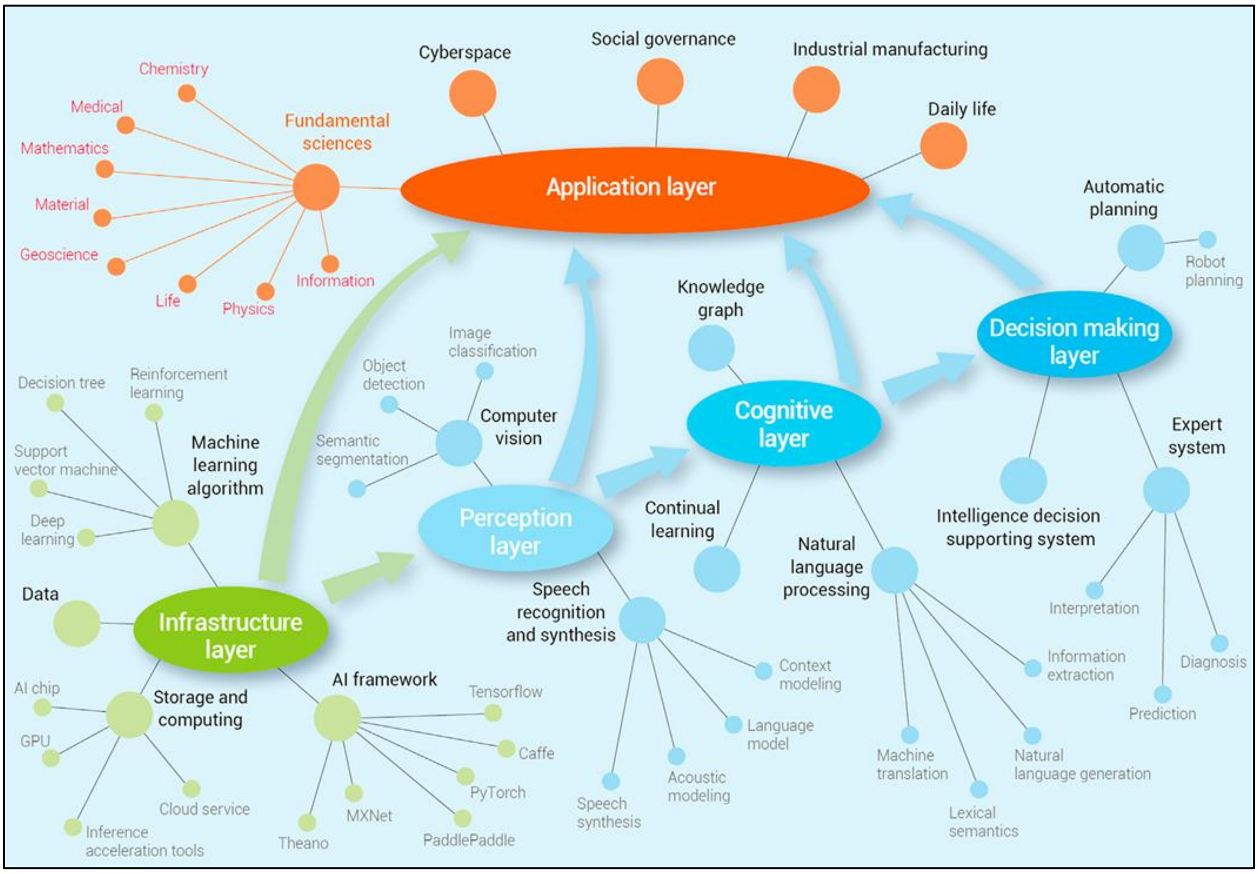


Figure 2 The knowledge graph of AI framework

Several trends are shaping the next generation of AI frameworks. One is the ability to train extremely large models efficiently across hundreds or thousands of devices, a need driven by Transformer-based models. Another is convergence toward more standardized APIs (for example, compatibility with NumPy-like interfaces). A third is better operator and kernel optimization so models can run efficiently on diverse hardware without hand-tuned, device-specific code.

2.3. AutoML: using AI to build AI

Automated machine learning (AutoML) aims to reduce manual effort in designing models and pipelines. One core idea is neural architecture search (NAS), which automates the discovery of network structures (X. Dong et al., 2024). NAS methods often use reinforcement learning, evolutionary strategies, or hybrids. In reinforcement-learning NAS, a controller proposes architectures, models are trained and evaluated, and performance feeds back as a reward signal (Alotaibi & Ahmed, 2025). Evolutionary NAS uses selection and mutation over a population of architectures. These approaches can produce competitive, sometimes state-of-the-art, architectures with less human trial-and-error.

2.4. AI-enabled networking under complex conditions

Modern networks operate in environments that are dynamic, heterogeneous, and difficult to capture with clean analytical models. DL and deep reinforcement learning can learn behaviors from data and adapt policies as conditions change (Singh et al., 2025). Potential applications span the protocol stack: physical-layer tasks such as interference management and modulation recognition; link-layer resource allocation and traffic prediction; routing optimization; and application-layer task scheduling or compression. Network security is also an important area, where ML can support anomaly detection and malicious-traffic classification (Kulin et al., 2021).

2.5. AI for nanophotonics and inverse design

Nanophotonic devices, including metasurfaces, often require solving Maxwell's equations in complex geometries a process that can become computationally expensive as designs grow in size and freedom. DL offers a data-driven shortcut for both forward prediction (estimating optical responses from structures) and inverse design (finding structures that match a desired response) (Lv et al., 2024). Researchers have used DNNs, CNNs, and hybrid CNN-RNN models to predict spectra from images of structures, and have applied supervised, unsupervised generative models, and reinforcement learning to propose new designs. Despite strong promise, interpretability—understanding why a model picks a design remains an open problem.

2.6. Additional directions

Beyond the examples above, AI is frequently proposed for predictive maintenance (risk monitoring from sensor streams), "digital twin" simulations for safer engineering analysis, intelligent robotics that adapts to changing environments, and AI-enabled IoT systems that sense and act in physical infrastructure (smart cities, transportation, utilities) (Javaid et al., 2023). These use cases elevate privacy and security concerns because they often involve personal and operational data.

2.7. AI in Mathematics

Mathematics underpins many classical AI methods k-nearest neighbors, support vector machines, and boosting are examples with strong theoretical roots. At the same time, the rise of DL has created new mathematical questions and renewed interest in topics such as optimization, probability, and function approximation (Xu et al., 2021).

2.8. Interpreting neural networks

From one perspective, ML builds nonlinear function approximators. Classic results such as universal approximation show that certain network families can approximate continuous functions under mild assumptions. Yet modern networks often succeed on tasks that look far beyond simple function classes, raising questions about what kinds of structures networks represent efficiently. Researchers therefore study the function spaces naturally linked to different architectures (e.g., kernel-based spaces, Barron-type spaces for two-layer networks, and other spaces proposed for deep or residual architectures) and analyze approximation error with quantitative norms.

2.9. AI in Medical Science

Healthcare is rapidly moving from basic digitization to connected services and, ultimately, "smart hospital" systems. As computing hardware and AI tools improve, algorithms for vision, language, and data mining are increasingly embedded in medical devices and clinical workflows (Rani et al., 2025).

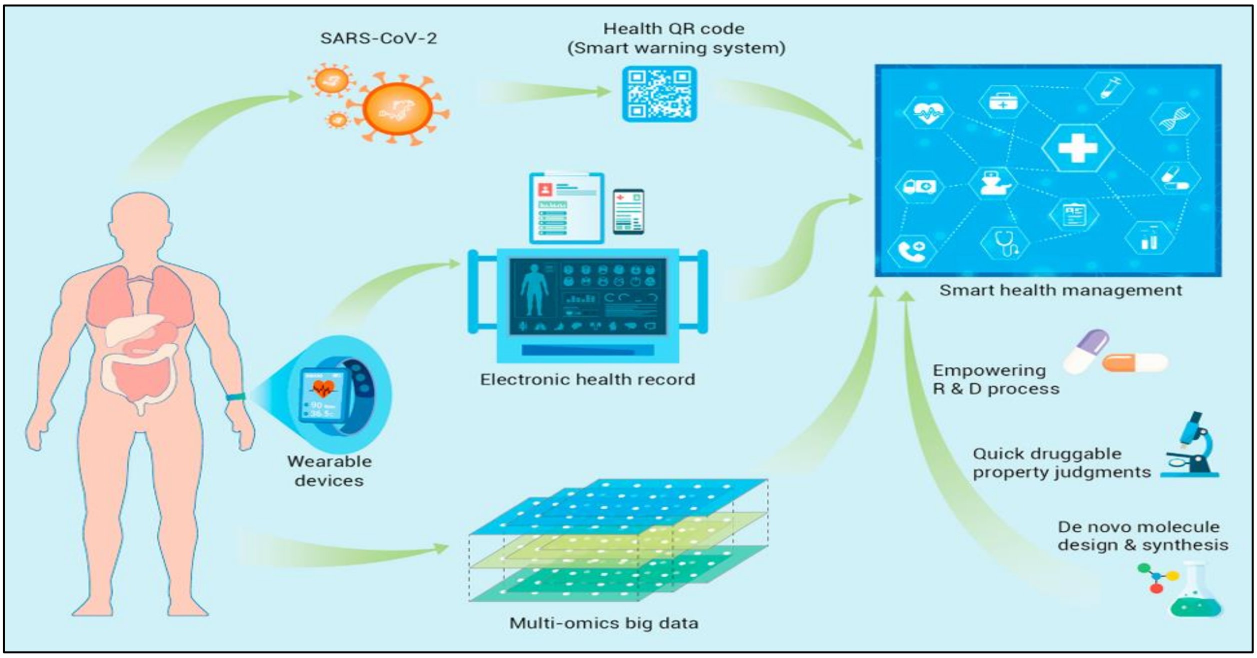


Figure 3 AI in medical sciences

2.10. Clinical decision support from records

Clinical decision support systems attempt to turn electronic medical records and biomedical literature into recommendations. IBM's Watson-based tools and other platforms have applied NLP to search case histories and publications, then propose and rank candidate treatment plans (Alexiuk et al., 2023). A common limitation is that recommendations may not transfer well across regions because they depend on local care practices, guidelines, and insurance policies. Many such systems also require continuous manual curation to keep their knowledge bases up to date.

2.11. Public health and outbreak monitoring

AI can assist public health by detecting outbreaks from heterogeneous signals such as search queries and social media. During COVID-19, some countries implemented digital health status systems that combined mobile data with risk scoring to support quarantine decisions and access control. These approaches can be effective at scale, but they also highlight trade-offs around privacy, transparency, and governance (Hammad, Rahamaddulla, Fauzi, et al., 2025; Villanueva-Miranda et al., 2025).

2.12. Biomarkers and predictive modeling

High-dimensional data multi-omics profiles, lab results, imaging, and patient demographics enable predictive models for diagnosis, prognosis, and treatment response. ML has been used to build severity predictors, drug-response models, and survival-risk tools across many cancer types. Common pipelines combine feature selection methods (e.g., LASSO) with statistical survival models such as Cox regression, sometimes augmented by DL representations (Babu & Snyder, 2023).

2.13. Medical imaging and devices

Medical imaging is one of the most mature areas of clinical AI, with extensive work on classification, detection, and segmentation. AI systems can reduce clinician workload and error by handling repetitive interpretation tasks consistently (Ogut, 2025). Examples include diabetic retinopathy screening tools approved by regulators, mobile applications for skin lesion assessment, ECG-based screening systems, and AI-assisted radiotherapy planning. Wearables and home devices add continuous monitoring; algorithms can flag early warning signals such as atrial fibrillation, and consumer genomics services can support individualized risk education and health planning.

2.14. AI-assisted drug discovery

Drug development is expensive and slow, often requiring years and large budgets to bring a compound to market. AI can speed up steps such as target identification, molecule generation, property prediction, and synthesis planning (Ahmad et al., 2026). A prominent example is protein structure prediction, where AlphaFold-style models substantially improved accuracy for many targets. Other platforms have reported rapid identification of candidate inhibitors and accelerated progression from design to early trials compared with traditional timelines (Borkakoti & Thornton, 2023). AI may also help reduce late-stage failures by improving early prediction of safety and efficacy risks.

2.15. Case example: cervical cancer workflows

Cervical cancer is often preventable and highly treatable when found early, yet screening quality can vary. Conventional workflows typically combine cytology, colposcopy, and histopathology (B. Dong et al., 2025). AI systems trained on large clinical and pathology datasets can help scale analysis, support clinicians in under-resourced settings, and provide prognostic tools that estimate recurrence risk and mortality informing postoperative decisions and follow-up planning.

2.16. AI in Materials Science

Materials are foundational to modern industry and emerging technologies. Historically, new materials were often discovered through slow trial-and-error experimentation or computationally expensive simulations (X. Jiang et al., 2025; Khan et al., 2025). As demands grow, AI offers a way to narrow the search space and prioritize promising candidates more efficiently.

2.17. AI in Geoscience

Geoscience problems climate impacts, air quality, natural hazard forecasting, water management, and energy systems have immediate societal relevance. New sensing technologies (e.g., satellites, remote platforms, and advanced drilling) and large simulations generate vast datasets, creating an opening for AI to help model Earth systems more effectively (Hammad, Rahamaddulla, Muhamad Tamyez, et al., 2025; D. Zhao, 2024).

Applying AI in geoscience is challenging because many phenomena have fuzzy boundaries in space and time, exhibit nonlinear multivariate behavior, and change over time (non-stationarity). Observations can be sparse, noisy, and uncertain, and labeled ground truth is often limited, especially for rare events (Gonzales-Inca et al., 2022).

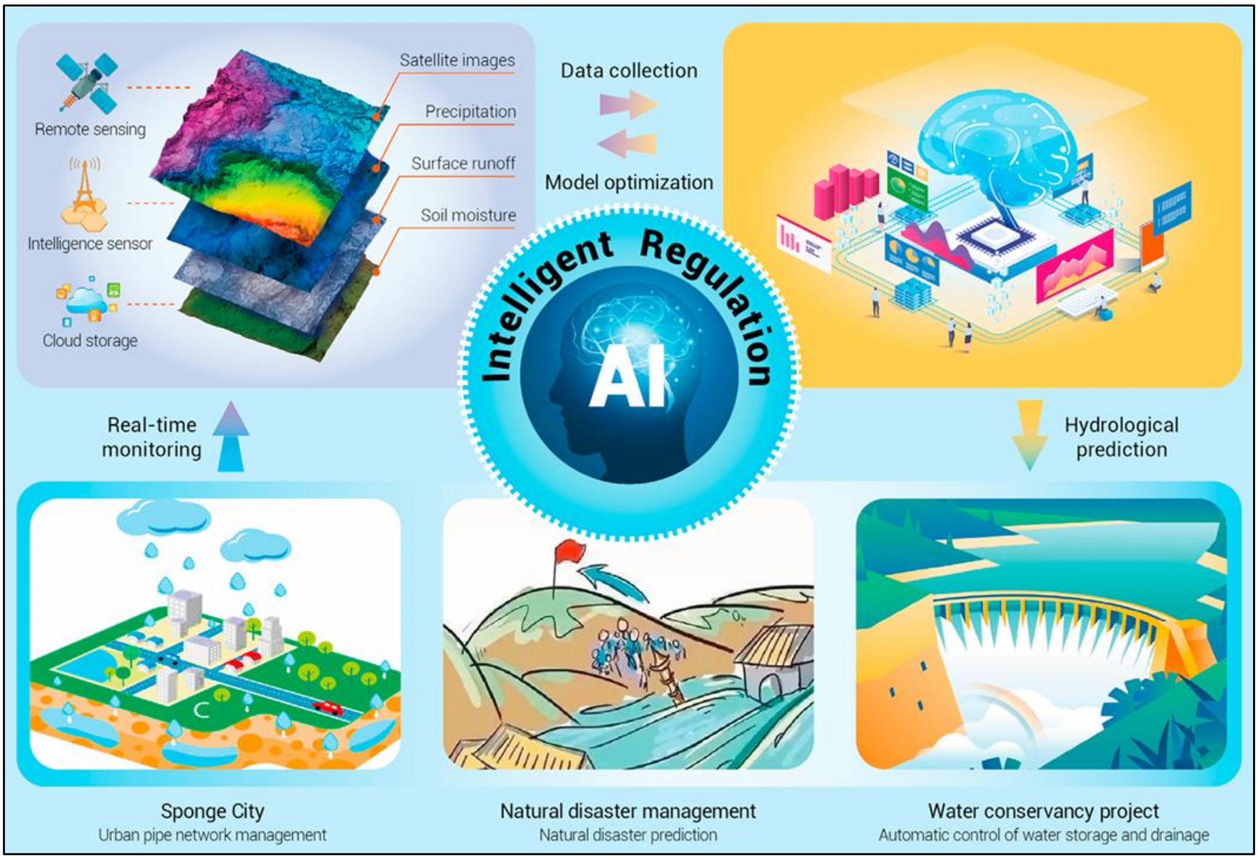


Figure 4 Applications of AI in hydraulic resource management

3. Where AI can help

AI methods can support (1) detecting and characterizing events and objects, (2) estimating variables from indirect measurements, (3) forecasting long-term trends from observational records, (4) discovering relationships among variables, and (5) causal attribution (Ahmed et al., 2020). These tasks often require models that explicitly handle uncertainty and spatiotemporal structure.

3.1. Resource management and energy systems

AI has been explored for urban water planning by forecasting demand and optimizing allocation to reduce cost and improve sustainability. In meteorology and environmental monitoring, ML can integrate multiple data sources to improve analysis of humidity, temperature, reef health, and other indicators. In energy systems, AI can help integrate renewable generation, optimize grid operation, reduce transmission losses, and identify inefficiencies, supporting decarbonization goals (Ferdowsi et al., 2024).

3.2. Collaboration and interpretability

Effective geoscience AI typically requires close collaboration between domain scientists and AI researchers, from defining questions and collecting samples to preprocessing and model selection. Interpretability matters because insights extracted from models can become scientific building blocks for understanding and prediction—not just black-box forecasts (T. Zhao et al., 2024).

3.3. AI in the Life Sciences

AI and biology influence one another. Many AI ideas were originally inspired by neuroscience, and AI is now a key tool for analyzing biological data at scale.

3.4. Mutual inspiration with neuroscience

Modern DL inherits ideas from neural computation, and many successful architectures reflect properties observed in biological vision systems (nonlinear processing, normalization, pooling) (Ekundayo & Ezugwu, 2025). Mechanisms analogous to attention and memory have improved performance on complex recognition problems. Conversely, AI provides formal models for testing hypotheses about learning and decision-making in the brain, for example, temporal-difference learning in reinforcement learning echoes patterns observed in neural reward signaling.

3.5. Omics, single-cell data, and protein structure

Genomics, epigenetics, proteomics, and single-cell sequencing now produce datasets too large and complex for manual analysis. AI can learn subtle patterns, support variant impact prediction, detect copy-number changes, and infer epigenetic modifications. In single-cell workflows, models can impute missing values, identify doublets, and learn developmental trajectories (Ren et al., 2025). Protein structure prediction has become a landmark success for DL, with AlphaFold-style models providing high-quality structures for large fractions of proteomes, an advance expected to accelerate drug discovery and functional biology.

3.6. Smart agriculture

Agriculture is moving toward “smart” systems that combine sensors, remote sensing, and ML. DL can support breeding by predicting candidate gene loci, transferring insights from well-studied species to less characterized crops, and modeling genotype-to-phenotype links for multi-trait improvement (Hammad, Fauzi, Tamyez, et al., 2025). In the field, data from satellites, drones, and portable devices can be fused to estimate crop health, nutrient stress, and yield, enabling more precise irrigation and fertilization decisions (Farooq et al., 2024). Computer vision models can assist with phenotyping, disease detection, and automated harvesting in dense environments.

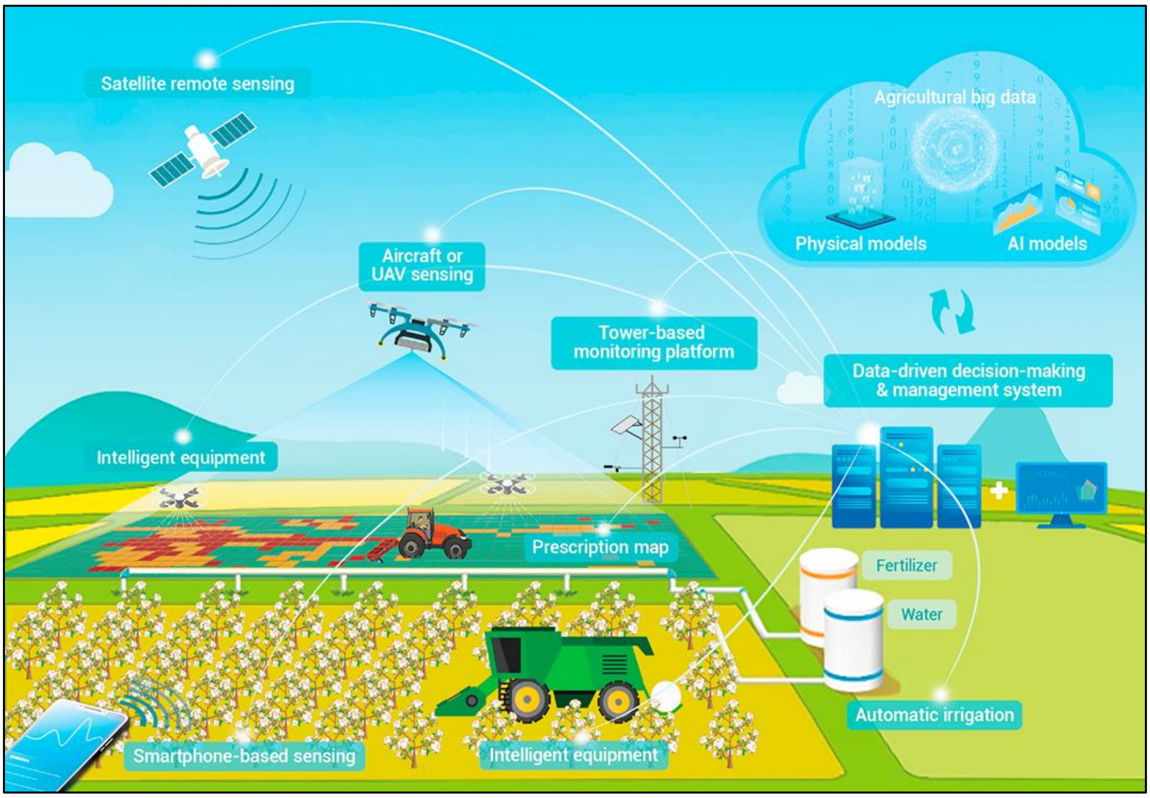


Figure 5 Integration of AI and remote sensing in smart agriculture

3.7. AI in Physics

Physics spans scales from subatomic particles to galaxies. Across this range, AI is increasingly used for data reconstruction, classification, and accelerating simulations.

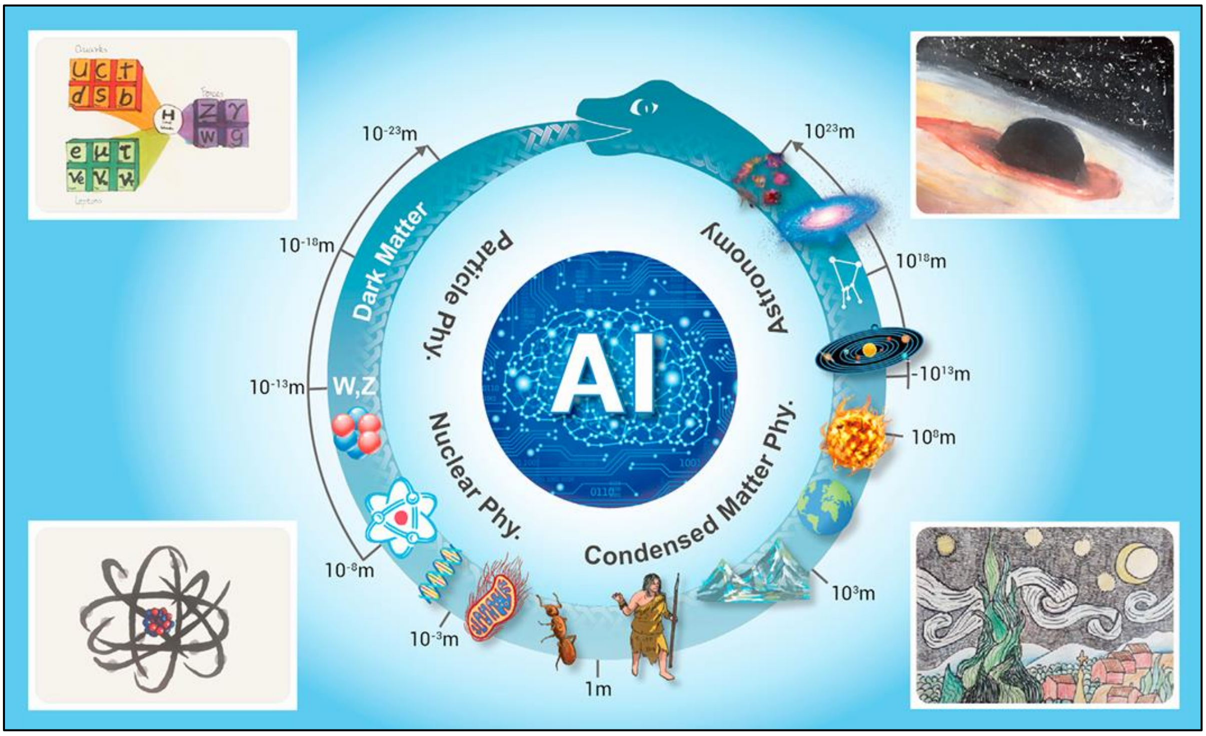


Figure 6 Scale of physics

3.8. Particle and nuclear physics

In lattice quantum chromodynamics, Markov-chain Monte Carlo simulations can suffer from slow mixing and topological freezing. ML methods have been explored to reduce variance, accelerate sampling, and improve the extraction of physical observables. In experiments, particle identification and track reconstruction benefit from classifiers and deep architectures such as U-Net for segmentation-like tasks. At large colliders, supervised ML helps distinguish rare signal events from overwhelming backgrounds, and quantum-enhanced ML ideas are being investigated for future workflows (Cranmer et al., 2023).

For nuclear detection and imaging, AI can help interpret complex signals (e.g., overlapping pulse shapes) that traditional methods handle poorly. Applications such as muon tomography leverage natural cosmic particles for non-destructive imaging and can be sped up by learned decision functions.

3.9. Condensed matter and materials modeling

ML has been used to improve electronic-structure modeling by tuning parameters (such as Hubbard U) and by learning improved energy functionals or kinetic energy approximations. Neural wavefunction methods demonstrate that AI can represent many-body quantum states with high accuracy in some settings (Cai et al., 2024). For molecular dynamics, learned interatomic potentials, kernel methods and neural message-passing models provide near-quantum accuracy at significantly reduced computational cost for many systems.

3.10. Astronomy and cosmology

Astronomy increasingly relies on automated analysis because modern surveys collect data at scales beyond what humans can label manually. DL is used for source detection, galaxy classification, transient event identification, and fast parameter inference (including real-time gravitational-wave signal decoding). Systems can automatically issue alerts, track fast-moving objects, and help construct more complete catalogs of the sky, enabling broader scientific discovery (Shao et al., 2026).

3.11. AI in Chemistry

Chemistry sits at the center of many sciences because it links structure, properties, and transformations of matter. Chemical knowledge is vast and continuously expanding, with databases cataloging hundreds of millions of substances and adding new entries daily. Because chemical and reaction spaces are effectively enormous, purely human exploration becomes infeasible; AI provides a practical route to navigate these spaces and discover useful patterns (Edwards et al., 2015).

3.12. Analytical and computational chemistry

In analytical chemistry, traditional feature selection depends heavily on expertise and can be biased or incomplete. DL can learn representations directly from spectroscopy and chromatography data, enabling faster and more objective interpretation (Gangwal & Lavecchia, 2025). For example, neural models can learn to classify Raman or SERS spectra and support accurate identification of analytes.

3.13. Synthesis planning, catalysis, and toxicology

In organic chemistry, supervised learning can map molecular structures to properties, and generative models can propose novel candidates by sampling chemical space. Retrosynthesis, once largely an art, can be supported by AI systems that plan routes and suggest viable reaction steps. When combined with robotics, these tools can enable automated, closed-loop synthesis and testing (Y. Jiang et al., 2023).

Catalyst discovery is another area where search spaces are huge, and performance depends on many coupled factors. ML, paired with high-throughput experimental and simulation data, can help identify descriptors that connect catalyst structure to activity, stability, and selectivity, supporting virtual screening and more targeted laboratory work (Fahima et al., 2025; Liu & Peng, 2024).

In toxicology and medical chemistry, predicting harm depends on many organism- and context-specific factors. Given the scope of required screening, AI is increasingly viewed as a realistic way to prioritize chemicals for testing and to support risk assessment while reducing ethical and practical burdens.

4. Conclusions and Outlook

Across fundamental disciplines, AI is changing how research is conducted: it can analyze high-volume data, propose hypotheses, accelerate simulations, and guide experiments. Despite rapid progress, several challenges remain.

Security and robustness are growing concerns. ML systems can be vulnerable to adversarial inputs, data poisoning, and model-level attacks such as backdoors, theft, inversion, or membership inference. Defenses exist, but attack methods evolve quickly, making robust system design an ongoing priority.

Another practical difficulty is dataset shift: training and deployment data may come from different distributions, and real-world patterns can drift over time. Updating models naively on new data can cause catastrophic forgetting, where past knowledge is overwritten. A major research direction is lifelong or continual learning moving from the classic pattern of offline training plus online inference to systems that can continuously learn while retaining and integrating prior skills. It carries out a comprehensive survey on the development and application of AI across a broad range of fundamental sciences, including information science, mathematics, medical science, materials science, geosciences, life science, physics, and chemistry. Despite the fact that AI has been pervasively used in a wide range of applications, there still exist ML security risks on data and ML models as attack targets during both training and execution phases. Firstly, since the performance of an ML system is highly dependent on the data used to train it, these input data are crucial for the security of the ML system. For instance, adversarial example attacks188 providing malicious input data often lead the ML system into making false judgments (predictions or categorizations) with small perturbations that are imperceptible to humans; data poisoning by intentionally manipulating raw, training, or testing data can result in a decrease in model accuracy or lead to other error-specific attack purposes. Secondly, ML model attacks include backdoor attack son DL, CNN, and federated learning that manipulate the model's parameters directly, as well as model stealing attacks, model inversion attacks, and membership inference attacks, which can steal the model parameters or leak the sensitive training data. While several defense techniques against these security threats have been proposed, new attack models that target ML systems are constantly emerging. Thus, it is necessary to address the problem of ML security and develop robust ML systems that remain effective under malicious attacks. Due to the data-driven character of the ML method, features of the training and testing data must be drawn from the same distribution, which is difficult to guarantee in practice. This is because, in practical application, the data source might be different from that in the training dataset. In addition, the data feature distribution may drift over time, which leads to a decline of the performance of the model. Moreover, if the model is trained with only new data, it will lead to catastrophic "forgetting" of the model, which means the model only remembers the new features and forgets the previously learned features. To solve this problem, more and more scholars pay attention on how to make the model have the ability of lifelong learning, that is, a change in the computing paradigm from "offline learning + online reasoning" to "online continuous learning," and thus give the model the ability of lifelong learning, just like a human being.

Compliance with ethical standards

Disclosure of conflict of interest

The authors hereby declare that there are no conflicts of interest in this research.

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