

AI-First Research Ecosystems: Redefining Multidisciplinary Innovation in the Digital Era

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Abstract: *Research organisations have so far adopted artificial intelligence (AI) in a piecemeal way: a literature tool here, a prediction model there, each attached to workflows that were designed for a pre-AI world. This paper argues that the next phase of multidisciplinary innovation depends on a different posture, which we call AI-first: research ecosystems in which data, models, workflows, people and rules are designed from the outset on the assumption that AI participates in every stage of inquiry. Writing from the combined perspectives of electronics and communication engineering, computer science, pharmacology and mathematics, we synthesise recent literature on AI-enabled discovery and on research and innovation ecosystems. We map the functions of AI across the research lifecycle, and propose the AI-First Research Ecosystem (AFRE) architecture comprising five interdependent layers: data commons, model and compute, agentic workflow, human expertise and collaboration, and governance and incentives, connected by explicit learning loops. Disciplinary vignettes show how each field both contributes to and draws from the shared layers. A five-level maturity model enables institutions to locate themselves between ad hoc tool use and a fully AI-first configuration, and five propositions are advanced for empirical testing. We also examine the guardrails—verification, provenance, authorship norms, equitable access to compute and protection against methodological monoculture—without which AI-first research would be faster but not better. The paper concludes with a staged roadmap for universities and research institutes, with specific reference to the Indian higher-education context.*

Keywords: AI-first research; research ecosystem; multidisciplinary innovation; AI for science; agentic workflows; FAIR data; maturity model; research integrity

I. INTRODUCTION

The organisation of research has been slow to change. Laboratories, departments, grant cycles and journals look much as they did several decades ago, even though the volume of literature, the dimensionality of data and the complexity of problems have grown enormously. Evidence suggests that this mismatch is costly. Research effort is rising while research productivity is falling (Bloom et al., 2020); the educational burden required to reach the frontier is increasing, pushing researchers into narrower specialisation and larger teams (Jones, 2009; Wuchty et al., 2007); and papers and patents have become less disruptive over time (Park et al., 2023). Meanwhile, the problems that societies most need solved—antimicrobial resistance, climate adaptation, resilient infrastructure, affordable health care—do not respect disciplinary boundaries.



Artificial intelligence (AI) is widely expected to ease these constraints. Reviews document its use for hypothesis generation, experimental design, and the collection and interpretation of large datasets across the sciences (Wang et al., 2023). Landmark results include accurate protein structure prediction (Jumper et al., 2021), the discovery of a new antibiotic candidate (Stokes et al., 2020), autonomous materials laboratories (Szymanski et al., 2023) and new results in pure mathematics obtained with machine guidance (Davies et al., 2021). A survey of more than 1,600 researchers conducted by *Nature* found that many expect AI tools to become very important or essential to their fields, while also expressing concern about misuse and over-reliance (Van Noorden & Perkel, 2023).

Most institutions, however, have adopted AI as an add-on. Individual researchers use a language model to summarise papers or a classifier to analyse images, but datasets remain siloed, compute is procured project by project, workflows are undocumented and policies on AI use are ambiguous. We describe this as an *AI-assisted* posture. An *AI-first* posture is qualitatively different: the ecosystem is designed on the assumption that AI will take part in every stage of research, so that data are machine-actionable by default, models and compute are shared infrastructure, workflows are orchestrated and logged, human roles are redefined around judgement and verification, and governance explicitly addresses AI. The phrase is borrowed from the technology industry, where Iansiti and Lakhani (2020) describe firms rebuilt around data and algorithms; our concern is what the analogous redesign means for research.

The paper pursues three objectives: (i) to clarify the concept of an AI-first research ecosystem and distinguish it from incremental adoption; (ii) to propose an architecture and a maturity model that institutions can use for diagnosis and planning; and (iii) to identify the guardrails necessary for AI-first research to remain trustworthy. The authorship team spans electronics and communication engineering, computer science, pharmacology and mathematics, and the paper draws on illustrative developments from each of these fields.

II. BACKGROUND

2.1 Research and innovation as ecosystems

The ecosystem metaphor emphasises interdependence among heterogeneous actors who jointly create value that none could create alone. Adner (2017) defines an ecosystem by the alignment structure of partners needed for a focal value proposition to materialise, and Jacobides et al. (2018) stress modularity and non-generic complementarities among participants. In research policy, related ideas appear in Mode 2 knowledge production, which is transdisciplinary and application-oriented (Gibbons et al., 1994), in the triple helix of university, industry and government (Etzkowitz & Leydesdorff, 2000), and in open innovation, where knowledge flows purposively across organisational boundaries (Chesbrough, 2003). The science-of-team-science literature adds that cross-disciplinary teams face substantial coordination costs related to language, method and credit (Stokols et al., 2008). An ecosystem view of AI-enabled research therefore directs attention to shared infrastructure, to interfaces between disciplines and to the rules that govern contribution and reward.

2.2 From the fourth paradigm to AI-enabled discovery

Hey et al. (2009) described data-intensive discovery as a fourth paradigm of science. AI extends it in three ways. First, representation learning extracts structure from unlabelled, multimodal data (LeCun et al., 2015), and foundation models can be adapted to many tasks with modest additional data (Bommasani et al., 2021). Second, AI can close the loop between hypothesis and experiment: the robot scientist concept (King et al., 2009) has matured into autonomous laboratories (Szymanski et al., 2023) and language-model agents that plan and execute experiments (Boiko et al., 2023). Third, AI may contribute to understanding as well as prediction; Krenn et al. (2022) distinguish AI as an instrument revealing otherwise hidden properties, as a source of inspiration for human scientists, and as a prospective agent of understanding. Kitano (2021) frames fully autonomous discovery as a grand challenge.

2.3 The gap

Existing work concentrates either on technical advances in AI for particular sciences or on generic models of innovation ecosystems. There is little guidance on how a research institution should be configured so that AI-enabled,



multidisciplinary work becomes routine, and even less on how to assess progress toward such a configuration. The architecture and maturity model proposed below address this gap.

III. APPROACH

The study is a conceptual synthesis based on an integrative review (Torraco, 2005; Snyder, 2019) and follows the theory-synthesis and model-building templates described by Jaakkola (2020). Literature was located through Scopus, Web of Science, IEEE Xplore, PubMed and Google Scholar using combinations of terms relating to AI (machine learning, deep learning, foundation models, large language models, autonomous laboratories) and to research organisation (research ecosystem, interdisciplinary, team science, open science, research infrastructure, research integrity). High-impact reviews, seminal technical papers and authoritative policy documents were prioritised. Each author reviewed the material relevant to his or her field and drafted a disciplinary vignette; the layers of the architecture were then derived inductively by identifying the resources and rules that recurred across vignettes. The paper reports no primary data, and empirical results mentioned are those of the cited authors.

IV. AI ACROSS THE RESEARCH LIFECYCLE

Table 1 maps the contribution of AI to six stages of the research lifecycle, together with the responsibilities that remain with human researchers. Two features deserve emphasis. The first is breadth: AI is relevant at every stage and not merely at the analysis stage where it first appeared. The second is that the human responsibilities in the right-hand column are not residual tasks but the locus of scientific accountability. Large language models can produce fluent text that is factually unsupported (Ji et al., 2023), and leading journals have stated that such tools do not satisfy the criteria for authorship and that their use must be disclosed (Nature, 2023). An AI-first ecosystem consequently increases the importance of verification skills.

Table 1. Functions of AI across the research lifecycle and retained human responsibilities

Lifecycle stage	AI functions	Illustrative sources	Retained human responsibility
Problem framing and literature synthesis	Semantic search; summarisation; mapping of latent connections across fields	Tshitoyan et al. (2019); Wang et al. (2023)	Judging significance; checking sources; identifying what is absent from the corpus
Hypothesis generation	Pattern discovery in data; candidate generation; conjecture suggestion	Davies et al. (2021); Stokes et al. (2020)	Assessing plausibility and mechanism; selecting hypotheses worth testing
Design of experiments and simulations	Active learning; surrogate models; planning by agents	Boiko et al. (2023); Karniadakis et al. (2021)	Safety and ethics approval; defining constraints and stopping rules
Data acquisition	Robotic execution; intelligent sensing; automated annotation	King et al. (2009); Szymanski et al. (2023)	Calibration; quality assurance; consent and privacy
Analysis and modelling	Representation learning; prediction; code generation	Jumper et al. (2021); Chen et al. (2021)	Validation design; guarding against leakage; interpretation
Reporting and translation	Drafting support; visualisation; translation into practice	Birhane et al. (2023); Nature (2023)	Authorship and accountability; disclosure of AI use; peer review

Source: Authors' synthesis of the cited literature.



V. THE AI-FIRST RESEARCH ECOSYSTEM (AFRE) ARCHITECTURE

Figure 1 presents the proposed architecture. Five layers are stacked in order of dependency and are connected by learning loops through which the outputs of research, including its failures, return as inputs.

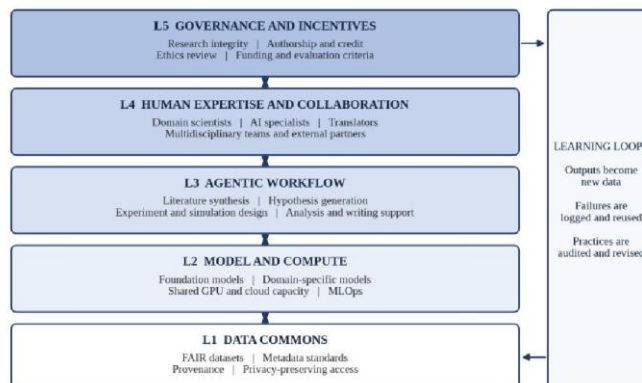


Figure 1. The AI-First Research Ecosystem (AFRE) architecture (authors' conceptualisation)

L1 Data commons. Data are treated as a shared institutional asset governed by the FAIR principles of findability, accessibility, interoperability and reusability (Wilkinson et al., 2016). Datasets carry documentation of provenance, composition and intended use (Gebu et al., 2021). Where data cannot be pooled, as with patient records, federated learning permits models to be trained across sites without moving the raw data (McMahan et al., 2017; Rieke et al., 2020).

L2 Model and compute. Foundation models, domain-specific models and accelerated computing are provisioned as common infrastructure and not purchased project by project. Models are documented with their evaluation conditions and limitations (Mitchell et al., 2019), and machine-learning operations practices are adopted to contain the hidden technical debt that accumulates in learning systems (Sculley et al., 2015).

L3 Agentic workflow. Research tasks are composed into orchestrated, logged pipelines in which AI agents retrieve literature, propose hypotheses, design experiments or simulations and draft analyses, with human checkpoints at defined stages. Logging makes each step auditable and reproducible, which is a condition for trusting results produced at machine speed.

L4 Human expertise and collaboration. Researchers' roles shift toward problem formulation, critical evaluation and integration across fields. A new boundary-spanning role—the translator who is fluent in both a domain and AI methods—reduces the coordination costs identified by Stokols et al. (2008). External partners in industry, hospitals and government participate through shared access to L1–L3.

L5 Governance and incentives. Policies cover research integrity, disclosure of AI use, authorship and credit, ethics review of AI-enabled studies and equitable allocation of compute. Evaluation and promotion criteria recognise datasets, software and models as research outputs, in line with international recommendations on open science (UNESCO, 2021).

Learning loops. In an AI-first ecosystem every project enriches the commons: new data flow back to L1, fine-tuned models to L2, reusable pipelines to L3, and lessons about failure to L5. Recording negative results is particularly valuable because models trained only on published successes inherit publication bias.

5.1 Propositions

P1. *Institutions with a mature data commons (L1) realise greater research benefit from a given investment in models and compute (L2) than institutions without one.*

P2. *Orchestrated and logged workflows (L3) increase the reproducibility of AI-enabled research relative to ad hoc tool use.*



P3. *The presence of boundary-spanning translators (L4) positively moderates the relationship between shared AI infrastructure and multidisciplinary research output.*

P4. *Explicit governance of AI use (L5) increases researchers' willingness to adopt AI and the external credibility of resulting outputs.*

P5. *Ecosystems with functioning learning loops improve more rapidly over time than ecosystems in which project outputs are not returned to the shared layers.*

VI. DISCIPLINARY VIGNETTES

6.1 Electronics and communication engineering

AI is reshaping both the design and the operation of electronic systems. O'Shea and Hoydis (2017) showed that a communication link can be represented as an autoencoder and optimised end to end, challenging the traditional block-by-block design of the physical layer. Reinforcement learning has produced chip floorplans comparable to those of expert designers in a fraction of the time (Mirhoseini et al., 2021). In the other direction, the discipline supplies the ecosystem with sensing hardware and with energy-efficient architectures for running deep networks on embedded devices (Sze et al., 2017), which determine what data can be collected in the field and at what cost.

6.2 Computer science and engineering

Computer science provides the methodological core, including learning algorithms, the transformer architecture (Vaswani et al., 2017) and the software infrastructure for training and deployment. Code-generating language models (Chen et al., 2021) lower the programming barrier for scientists in other fields, which is itself a mechanism of multidisciplinary integration. The discipline also contributes privacy-preserving computation (McMahan et al., 2017) and engineering discipline for machine-learning systems (Sculley et al., 2015). In return it receives demanding real-world problems and datasets that expose the limits of methods developed on benchmarks.

6.3 Pharmacology and medicine

Machine learning is applied throughout drug discovery and development, from target identification and molecular design to biomarker discovery and trial analysis (Vamathevan et al., 2019). Stokes et al. (2020) used a deep network to screen chemical libraries and identified a compound with antibacterial activity structurally distinct from known antibiotics, and structure prediction (Jumper et al., 2021) has become a routine input to target analysis. Clinical deployment requires rigorous validation and attention to workflow and bias (Topol, 2019). Pharmacology contributes to the ecosystem high-value experimental and clinical data, a mature culture of ethics review and regulatory-grade standards of evidence that other AI-using fields can emulate.

6.4 Mathematics

Mathematics supplies the foundations of learning—optimisation, probability, linear algebra and approximation theory—and increasingly benefits from AI in return. Davies et al. (2021) used machine learning to detect patterns that guided mathematicians to new results in knot theory and representation theory. Program search with large language models has yielded new constructions for open problems in combinatorics (Romera-Paredes et al., 2024), and a neuro-symbolic system has solved olympiad-level geometry problems (Trinh et al., 2024). Physics-informed neural networks embed differential equations in the training objective (Raissi et al., 2019), connecting mathematical modelling to the data-driven methods used by engineers and, potentially, to mechanistic modelling in pharmacology.

6.5 Convergence

Table 2 summarises the exchanges. The same shared layers serve all four fields, and each field's contribution becomes another's input: sensors designed by engineers produce data for pharmacologists; mathematical constraints improve the models of both; software tools make all of it accessible. This pattern of reciprocal, non-generic complementarity is what distinguishes an ecosystem from a collection of projects (Jacobides et al., 2018).



Table 2. Reciprocal contributions of four disciplines within an AI-first ecosystem

Discipline	Contributes to the ecosystem	Receives from the ecosystem
Electronics and communication engineering	Sensors and instrumentation; edge and low-power AI hardware; signal-processing expertise	Learned design automation; end-to-end optimisation methods; application problems from health and environment
Computer science and engineering	Algorithms and architectures; MLOps and software tooling; privacy-preserving computation	Challenging real-world datasets; domain constraints that expose limits of benchmark-driven methods
Pharmacology and medicine	Experimental and clinical data; ethics and regulatory standards; validation culture	Candidate generation and screening; structure prediction; federated analytics across hospitals
Mathematics	Optimisation, statistics and modelling foundations; guarantees and uncertainty quantification	Pattern discovery for conjectures; program search; computational experimentation at scale

Source: Authors' conceptualisation.

VII. A MATURITY MODEL FOR AI-FIRST RESEARCH

Institutions differ widely in resources and starting points. Table 3 sets out a five-level maturity model that can be used for self-assessment. The levels are cumulative, and the model is descriptive: it is intended to structure discussion and planning and has not yet been validated as a measurement instrument.

Table 3. Five-level maturity model for AI-first research ecosystems

Level	Data and infrastructure	Workflow	People and collaboration	Governance
1. Ad hoc	Data on personal devices; no shared compute	Individual use of public AI tools	Isolated enthusiasts	No policy on AI use
2. Assisted	Departmental repositories; occasional cloud credits	AI used for discrete tasks such as search and analysis	Informal peer support; short workshops	Basic guidance on disclosure and plagiarism
3. Integrated	Institutional repository with metadata standards; shared GPU facility	Documented pipelines within projects	Cross-department projects; research software support	Policy on AI use, data management and authorship
4. Orchestrated	FAIR data commons; model registry; federated links to partners	Logged agentic workflows with human checkpoints	Translator roles; joint appointments; industry and hospital partners	AI-specific ethics review; audit of reproducibility



Level	Data and infrastructure	Workflow	People and collaboration	Governance
5. AI-first	Machine-actionable data by default; continuous curation	Closed-loop experimentation where appropriate; reusable workflow library	Roles, training and curricula redesigned around human–AI collaboration	Incentives reward data, software and negative results; learning loops institutionalised

Source: Authors' conceptualisation.

VIII. RISKS AND GUARDRAILS

An AI-first ecosystem amplifies weaknesses as readily as strengths. Five risks require explicit guardrails.

- **Invalid results at scale.** Data leakage and related errors have been documented across many fields that use machine learning and typically inflate reported performance (Kapoor & Narayanan, 2023). Guardrails include pre-specified validation protocols, independent replication and logged workflows.
- **Fabrication and unverifiable text.** Generative models may produce plausible but unsupported statements (Ji et al., 2023). Every AI-generated claim, citation and number should be traceable to a verifiable source, and AI use should be disclosed (Nature, 2023).
- **Methodological monoculture and illusions of understanding.** Messeri and Crockett (2024) caution that AI tools may narrow the range of questions asked and methods used, while giving researchers the impression of understanding more than they do. Ecosystems should protect methodological plurality and theory-driven inquiry.
- **Compute and data divides.** The resources for frontier AI are concentrated in industry (Ahmed et al., 2023). Shared national and consortium facilities, open models and efficient methods reduce the risk that AI-first research is confined to a few institutions.
- **Environmental cost and deskilling.** Training large models consumes significant energy (Strubell et al., 2019), and routine delegation may erode foundational skills among early-career researchers. Reporting of computational cost and curricula that teach fundamentals before automation are appropriate responses.

IX. IMPLICATIONS AND ROADMAP

For institutional leaders, the architecture implies a sequence. Investment in the data commons and in governance should precede or accompany investment in models and compute, because the latter deliver little without the former. A staged roadmap may be outlined as follows: in the first year, adopt a policy on AI use and data management, audit existing datasets and establish a shared compute allocation; in the second year, build an institutional repository with metadata standards, appoint research software engineers and translators, and launch cross-department seed projects around societal problems; in the third year and beyond, introduce logged workflow platforms, federated partnerships with hospitals and industry, and revised evaluation criteria that recognise datasets, software and negative results.

For Indian higher education, the policy context is favourable. The National Education Policy 2020 calls for multidisciplinary institutions and a stronger research culture (Ministry of Education, 2020), and recent national initiatives on research funding and AI infrastructure are intended to widen access to resources beyond a small number of elite institutions. State engineering colleges, affiliated institutes and medical institutes can participate in AI-first ecosystems through consortia that share L1–L3 resources, even where no single member could sustain them alone. For funders, the implication is to support shared infrastructure and boundary-spanning roles and to require data and model documentation as a condition of funding.



X. LIMITATIONS AND FUTURE RESEARCH

The paper is conceptual. The vignettes reflect the disciplines of the authors and do not cover the social sciences, arts or humanities, where AI-first research raises distinct questions. The maturity model requires validation. Future work should develop indicators for each layer, apply the model in multi-institution case studies, test the propositions with longitudinal bibliometric and survey data, and evaluate interventions such as translator roles and logged workflow platforms through quasi-experimental designs.

XI. CONCLUSION

Adding AI tools to research systems designed for an earlier era yields incremental gains. Redefining multidisciplinary innovation requires AI-first ecosystems in which shared data, shared models, orchestrated workflows, redefined human roles and explicit governance are designed together and connected by learning loops. The AFRE architecture and maturity model offered here provide a vocabulary and a diagnostic for that redesign. The vignettes from engineering, computing, pharmacology and mathematics show that the same shared layers can serve very different fields and that each field's outputs become inputs for the others. The guardrails matter as much as the infrastructure: an AI-first ecosystem that cannot verify, reproduce and fairly attribute its results would simply generate unreliable knowledge more quickly. Designed with care, it offers a realistic route to research that is faster, more integrative and more widely accessible.

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