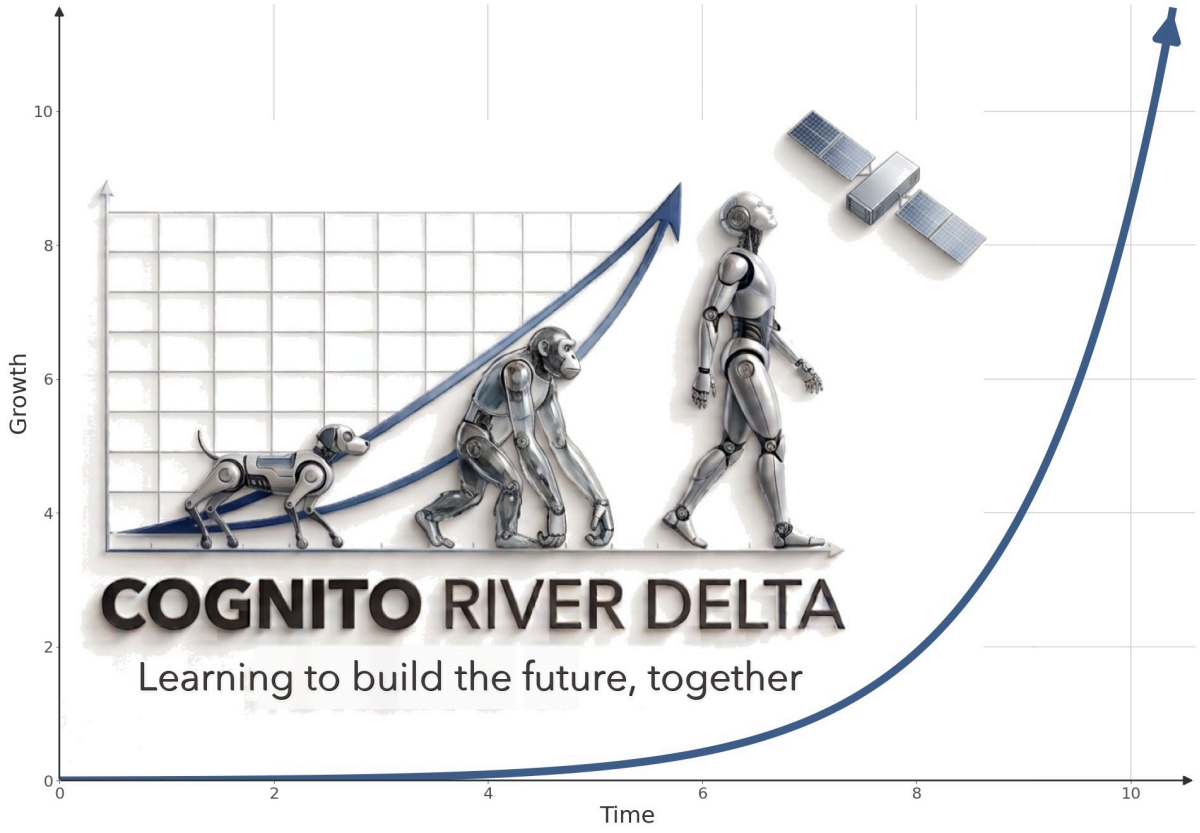


CATEGORY ROLLUP

AI for science - 2026-W46

Week of November 9, 2026

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Week of November 9, 2026 · 9 min read

AI for science

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Overview

The central storyline of this week in the AI for science (AI4S) sector is an escalating tension between two fundamentally different philosophies of progress: a "scaling-first" approach, which seeks to unlock new scientific frontiers through mathematical complexity and massive datasets, and a "grounding-first" approach, which insists that AI remains a secondary tool that must remain tethered to physical reality and fundamental laws. This week's developments highlight a field that is moving past the initial "wow factor" of protein folding and is now grappling with the much harder problems of biological intervention, the mathematical limits of scaling, and the "validation gap" between digital prediction and physical reality.

On one side, we see a push toward deeper mathematical rigor. Researchers like Surya Ganguli are attempting to move the field away from empirical "trial and error" scaling by applying statistical mechanics and high-dimensional geometry to derive first-principles models of how AI learns. This is a quest to understand the "how" of intelligence. On the other side, we see a pragmatic, application-driven insistence that even the most sophisticated generative models —such as those used for enzyme engineering—cannot bypass the necessity of the physical laboratory. Aubrey de Grey’s work in biological engineering underscores that while AI can design the molecules required for complex repairs, the ultimate arbiter of truth remains the wet lab.

The week’s insights suggest that the "next big thing" in AI4S is not merely a more powerful model, but the successful integration of these two forces: creating AI that is mathematically

capable of exponential scaling while remaining strictly constrained by the unyielding laws of biology and physics. This tension is driving a fundamental shift in scientific methodology: the transition from traditional, slow-moving numerical simulations (such as classical molecular dynamics) to rapid, machine-learning-driven surrogate modeling. As AI becomes the "engine" of discovery, the focus of the sector is shifting from asking "what does this molecule look like?" to "how can we engineer a biological system to behave in a specific way?"

AI for Science

The current state of AI for science is defined by a pivot from passive observation—predicting how a system behaves—to active engineering—designing the components of those systems. This shift is most visible in two distinct but converging domains: the structural biology of disease and the mathematical theory of AI scaling.

The Biological Engineering Frontier

In the realm of biotechnology, the conversation has moved significantly beyond the foundational success of AlphaFold and ESMFold. While the ability to predict protein structures and macromolecular complexes was a landmark achievement that transformed structural biology from an experimental bottleneck into a computational data-fetching step, the current frontier is the use of these models to engineer functional biological tools.

Aubrey de Grey’s recent focus highlights this leap in utility. We are seeing a move from mapping the "parts list" of life to designing the "tools" that can manipulate those parts. Specifically, de Grey notes that AI is being deployed to engineer the specific enzymes and molecules required for complex biological repairs, particularly within the framework of SENS-based (Strategies for Engineered Negligible Senescence) interventions. This includes designing molecules capable of removing intracellular waste and breaking down the crosslinks in the extracellular matrix—processes that are central to addressing the mechanisms of biological aging.

However, this frontier faces a persistent and critical bottleneck: the "validation gap." Despite the power of generative models to hypothesize an enzyme that can break down a specific crosslink, the actual verification of that enzyme's efficacy, safety, and stability must still occur through physical biological experimentation. This dependency is a primary driver for the industry's move toward "Autonomous Laboratories" (or self-driving labs). These systems aim

to bridge the gap between computational design and physical execution by combining robotic synthesis with Bayesian optimization and active learning, allowing for an iterative loop where AI formulates hypotheses and executes physical lab work without constant human intervention.

The Mathematical and Scaling Frontier

While biologists are focusing on the "what" of biological engineering, theorists are focusing on the "how" of model capability. The central question is whether current AI scaling laws will eventually hit a wall or if there is a path to true exponential progress. Surya Ganguli is addressing this by moving away from the empirical "trial and error" approach to scaling and toward first-principles mathematical models derived from statistical mechanics and high-dimensional geometry.

A major hurdle in the field is the "Out-of-Distribution (OOD) generalization" problem. Current scientific AI models are often excellent at interpolating within known data but struggle when tasked with predicting entirely novel chemical spaces, extreme phase transitions, or rare physical phenomena. To solve this, Ganguli has proposed the use of "black swan" datasets—outlier data points representing rare or extreme phenomena. The theory is that by training on these high-information "black swans," models can achieve exponential rather than merely polynomial scaling, gaining the ability to predict breakthroughs rather than just interpolating existing knowledge.

Furthermore, Ganguli’s work on "digital twins" of neural circuits represents a sophisticated attempt to bridge the gap between artificial and biological intelligence. By creating high-fidelity mathematical simulations of biological neural processes, researchers hope to create a feedback loop where AI can learn from the very biological structures it is meant to model. This is an attempt to move AI from a "black box" surrogate model to a mathematically transparent system.

This mathematical rigor is also being applied to the growing risk of emergent behavior in multi-agent systems. As AI agents begin to work together in autonomous labs or complex simulations, the need for "safety-first architectures" becomes paramount. Ganguli’s focus on ensuring these systems are mathematically grounded from the start is a direct response to the inherent instability and unpredictability that can arise from unconstrained scaling.

Cross-cutting themes

The most significant theme emerging this week is the **Convergence of Simulation and Reality**. There is a clear, multifaceted effort to close the loop between digital prediction and physical manifestation. This is not happening in a single venue but in a hybrid space between high-performance computing (HPC) clusters and robotic synthesis labs. We see this in de Grey's focus on using AI for physical repairs, Ganguli's work on digital twins of biological circuits, and the broader industry move toward autonomous, robotic laboratories. The "science" is increasingly defined by how effectively a model can transition from a digital surrogate to a physical reality.

A second theme is the **Shift from Quantity to Quality of Data**. The traditional "more is better" approach to training data is being challenged by the realities of scientific discovery. While conversational AI thrives on massive text corpora, scientific AI faces "data scarcity," where high-fidelity data is often siloed, proprietary, or noisy. Whether it is the need for "black swan" datasets to drive exponential scaling (as proposed by Ganguli) or the struggle with noisy data in materials science, the consensus is shifting toward the idea that the next generation of scientific AI will be defined by its ability to learn from *meaningful* data—data that contains the rare, high-information physics or biology that typical datasets miss.

Finally, there is the **Integration of Physical Laws into Model Architecture**. To prevent the "black box" problem where purely data-driven models violate fundamental laws—such as the conservation of energy or mass—the field is seeing a rise in Physics-Informed Neural Networks (PINNs). This represents a critical attempt to bake governing physical laws directly into the loss functions of models. This "mathematical grounding" is required to ensure that an AI-designed enzyme (as discussed by de Grey) or an AI-simulated neural circuit (as discussed by Ganguli) remains physically viable.

Where sources agree

- **The End of the Structural Biology Bottleneck:** There is a consensus that AI (specifically the AlphaFold and ESMFold series) has fundamentally transformed structural biology, moving it from a slow, experimental hurdle to a rapid, computational data-fetching step.
- **The Necessity of High-Fidelity Data:** Both the theoretical and applied perspectives suggest that the volume of data is becoming less important than its quality and

"extremity." For both scaling (Ganguli) and engineering (de Grey), the ability to handle rare or complex phenomena is the true frontier.
- **The Role of AI as an Accelerator, Not a Replacement:** Even the most advanced proponents of AI-driven discovery acknowledge that physical reality—whether through manual experimentation or robotic autonomous labs—remains the ultimate arbiter of scientific truth.

Where sources disagree

- **The Path to Scaling:** There is an implicit tension regarding the primary driver of the next leap in intelligence. Does it come from the "safety-first," mathematically structured architectures and "black swan" data strategies proposed by Ganguli, or does it come from the brute-force application of AI to existing biological datasets to find new functional patterns, as implied by de Grey's work in enzyme engineering?
- **The Level of Autonomy Required:** There is a divergence in the perceived necessity of human involvement. While the background suggests a trajectory toward fully "autonomous laboratories," de Grey's emphasis on the indispensable nature of physical experimentation suggests a more cautious, perhaps more supervised, iterative process where the human remains a critical part of the validation loop.

Numbers and claims to verify

- **The "Black Swan" Scaling Claim:** Can the use of "black swan" datasets, as proposed by Surya Ganguli, actually move model scaling from polynomial to exponential?
- **Enzyme Engineering Efficacy:** To what extent can current models like AlphaFold be utilized to design *entirely new* enzymes for SENS-based repairs, as opposed to simply predicting the structure of known sequences?
- **Surrogate Model Speedup:** The claim that neural operators (such as Fourier Neural Operators (FNOs) and Graph Neural Networks (GNNs)) can approximate partial differential equations (PDEs) "orders of magnitude" faster than traditional HPC solvers requires empirical verification in specific scientific use cases.

Investment and strategic implications

- **The "Hardware-Software Convergence" Investment:** Strategic value is migrating toward companies that can bridge the gap between AI software and physical hardware. This includes the providers of "Self-Driving Labs" (combining robotics with Bayesian optimization) and the developers of specialized mixed-precision hardware required for the convergence of traditional simulation and deep learning, such as the architectures used in exascale supercomputers like Frontier and Aurora.
- **The Rise of "Physics-First" AI Startups:** There is a growing strategic opportunity in companies building "Physics-Informed" models (PINNs). In high-stakes fields like drug discovery and materials science, the ability to guarantee that a model adheres to conservation laws is a massive competitive advantage over purely data-driven "black box" competitors.
- **Data as a Moat:** In an era where general-purpose AI is becoming commoditized, the true competitive "moat" for scientific AI companies will be access to high-fidelity, proprietary, and "black swan" datasets that are not available in the public domain.

What to watch next week

- **New benchmarks for PINNs:** Look for research or technical announcements regarding the accuracy and speed of Physics-Informed Neural Networks compared to traditional numerical solvers in fluid dynamics or molecular modeling.
- **Developments in "Digital Twins":** Watch for news regarding the scaling of digital twin simulations for complex biological systems or the integration of these twins into larger multi-agent research frameworks.
- **Autonomous Lab Milestones:** Monitor for any reports on the successful integration of large language models (LLMs) into robotic chemical synthesis workflows or autonomous hypothesis-generation loops.

Appendix: Individual perspectives

We see further because we stand on the shoulders of giants. The people in this appendix are some of those giants: their public work, followed and studied every day and every week, is how CognitoRiverDelta brings the world's AI knowledge and concerns together, so that, in

time, our expert panel can help shape real solutions and paths forward for all of us. We learn by observing them, and we think of them as kindred spirits: people helping humanity and AI educate each other and contribute to solutions. Together they form a much larger community of minds, a worldwide panel; ours is a small copy of it. Most people don't want to become expert kayakers, reading rocks and rapids every day; yet that is how this fast-flowing river of change feels to many of us, and the evidence that could ease those fears, the grounded ones and the imagined ones, is still being gathered. That is the work. We credit their ideas here with gratitude; they are not affiliated with us and do not endorse this report.

- **Aubrey de Grey**: Views AI as a critical tool for accelerating drug discovery and biological engineering (specifically for SENS-based repairs like removing intracellular waste and breaking down extracellular matrix crosslinks), but maintains that physical biological experimentation remains a non-negotiable requirement for scientific truth.
- **Surya Ganguli**: Advocates for a mathematically rigorous approach to AI, using statistical mechanics and high-dimensional geometry to understand scaling. Proposes "black swan" datasets for better scaling, "safety-first" architectures for multi-agent systems, and the use of "digital twins" to bridge the gap between biological and artificial intelligence.

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AI for science - 2026-W45

The central tension in the scientific landscape this week lies in the widening gap between the "digital promise" of simulation and the "biological reality" of the laboratory. We are witnessing a fundamental shift in how

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