Revolution of Scientific Inquiry in the age of AI

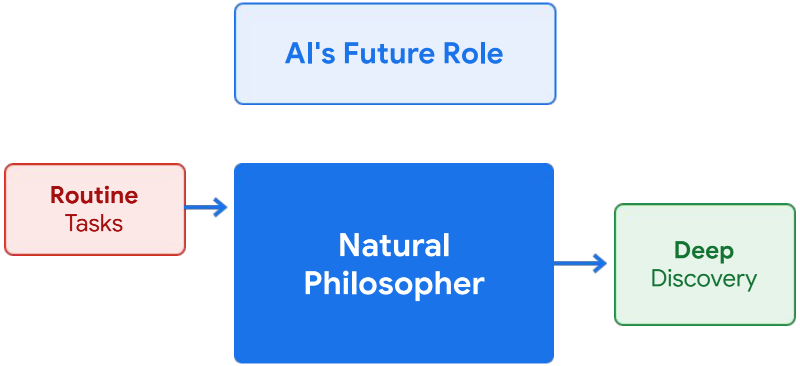
The Evolving Landscape

AI has transitioned from pattern matching to an active participant in discovery.

The shift necessitates reflection on the role of science for achieving human goals.

The Two Pillars of Science

- **Philosophy:** Satisfying curiosity and human understanding.
- **Engineering:** Predicting real-world outcomes through
    - Prediction (if this happens, then what else will happen)
    - Inference (if i saw this happen, what else must have happened / be true)
    - Design (choose actions/design devices to achieve given outcome)



The Synthesis

AI will take over routine tasks, allowing scientists to focus on distilling reality into the simplest, most powerful approximations of nature.

Scientific Models: Low-Dimensional Approximations

Core Principles

Approximation: Science creates simplified, computable versions of reality (e.g., Newton's laws, Maxwells eqns, predator-prey models).

Evolution: Shift from mechanistic models to predictive, non-explanatory ones (e.g., Descartes' fluid model of gravity to Newton's unmechanistic model).

Hierarchy: Multi-scale models focused on specific domains of space, time, and energy.

The Scientist's Mandate

- Design approximations capturing only essential dynamics.
- Maximize predictive power and range of applicability (avoid overfitting)

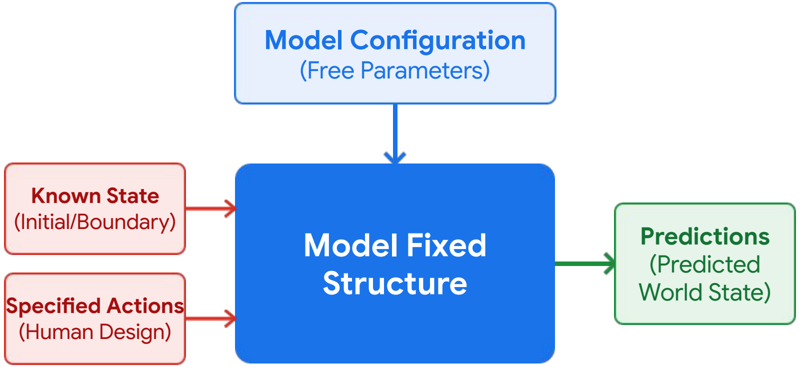
The "Crank Box": Model Structure and Utility

Core Concept

A model is a functional "crank box" blending fixed logic with configurable parameters.

Operational Modes

- **Prediction:** Forecast future actions based on current state and proposed human input.
- **Inference:** Reconstruct initial states from observed outcomes and actions.
- **Optimization:** Identify optimal actions to reach a specific target state.



Information Flow Summary

Models integrate external world inputs and controlled human actions to generate predictions about the world state.

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Cross-Domain Layering

Ecological Modeling

Uses aggregate metrics to model complex ecosystems, informed by individual organism structure.

Organism Modeling

Treats fluids major organs and flows of material and signals between them, ignoring the chemical dynamics of these interactions.

Fluid Dynamics

Treats fluids as continuous substances, intentionally ignoring discrete molecular reality for tractability.

Molecular dynamics

Models atoms as independent entities that affect each other by pair-wise forces, ignores quantum fields.

AI as a New Tool in Modeling

Neural Modeling

Configurable Components

- Simple fixed structures with many configurable components.
- Captures complex dynamics into low-dimensional representations.
- Requires extensive data for training.

Structured Modeling

Fixed Components

- LLMs generate and evolve PDEs as Python code via error feedback.
- Ideal for data-limited domains requiring strong inductive bias.

Hybrids combine neural models with physics-based constraints.

AI provides "new hammers" for the model-building approach.

The Enduring Role of the Human Scientist

The New Paradigm

AI as the Developer

- AI is replacing human model developers, mirroring how electronic computers replaced human computers in the 1940s.
- The shift returns scientists to their roots as natural philosophers, assisted by AI tools.

Human Value

Philosophical Distillation

- The core job is distilling primary drivers of behavior from the real world.
- Combining observation and data to create the simplest, tractable approximation of reality.

Humans define the "what" and "why," while AI handles the "how."

The scientist's value remains in identifying the essential dynamics of the real world.

Greg Bronevetsky works at the intersection of machine learning and scientific modeling. He received his PhD in Computer from Cornell University in 2006 and subsequently worked at Lawrence Livermore National Laboratory as a Lawrence Post-doctoral Fellow and then Member of Technical Staff until 2015. During this time he conducted research on the design of high-performance and resilient computing systems. Greg has worked in various roles across Alphabet since 2015 and is currently an engineer at X, The Moonshot Factory, where he focuses on scientific modeling and its applications. Greg is the recipient of the 2010 Presidential Early Career Award for Scientists and Engineers (PECASE).