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Simulation intelligence: A novel paradigm for simulation research in the era of Artificial Intelligence

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Simulation has long served as a foundational methodology in scientific inquiry, valued for its controllable, repeatable, and predictable nature across fields ranging from particle dynamics, fluid computation to social system analysis. However, under the profound impact of Artificial Intelligence (AI), the classical discipline of simulation faces profound conceptual and practical challenges: (1) How does similarity principle work in modeling complex system? (2) Are physics-based models still the optimal modeling approach? (3) How to understand "World Model" in simulation discipline? (4) What is the ultimate purpose of simulation experiments? (5) Does the top-down simulation system engineering remain effective? In this context, questions such as "Can simulation still stand as an independent methodology?" are being raised across scientific and engineering communities. To address these concerns from a broader perspective: Simulation Intelligence is proposed to revolutionize the traditional simulation research methodology. As a result, the traditional foundations of simulation are reconceptualized below.

THE DEFINITION OF SIMULATION INTELLIGENCE

Simulation Intelligence is a novel research paradigm that bridges data-driven and physics-based modeling approach, leveraging artificial neural networks to refine the fundamental Similarity Principle. Unlike traditional simulation, which relies primarily on explicit physical equations and top-down design, Simulation Intelligence utilizes "Intelligent Surrogate Models" to learn system dynamics from data.[1] Distinct from Artificial General Intelligence (AGI), which seeks universal cognitive capabilities, Simulation Intelligence is domain-specific, driven by a closed-loop framework of Forward Design and Inverse Modeling, focusing on constructing high-fidelity, evolvable virtual environments ("World Model") to enable Generative Computational Experimentation to support the training of intelligent agents (Figure 1).

THE SIMILARITY PRINCIPLE OF SIMULATION INTELLIGENCE: FROM MECHANISTIC SIMILARITY TO CONNECTIONISM

The similarity principle has long served as the foundational premise for model construction in traditional simulation disciplines. From geometric scaling to behavioral analogy, the similarity principle plays an important role in each research domain. However, the meaning of "similarity" varies dramatically across disciplines: it may refer to appearance similarity, functional equivalence, or perception correspondence. Lacking a unified theoretical foundation, the dilemma of "multiple explanations in different scenario respectively" is often faced.

To address the challenge, it is necessary to establish a new connection-based modeling view for simulation. This perspective moves beyond the general system theory, employing graph theory and data-driven techniques to represent reality as a network of agents, connections, and organizations. It enables the natural emergence of system behavior through the rules governing interactions among agents. Consequently, the Similarity Principle evolves from mechanistic similarity to connectionism, and from static mapping to evolutionary construction. As a result, it brings the emergence of "Simulation Intelligence". In this paradigm, the artificial neural network based "Intelligent Surrogate Models" serve as the fundamental units for modeling, "World Model" is the key part of the simulation system. "Model Training", "Generative Computational Experimentation" and "Forward Design and Inverse Modeling" are the kernel activities in the simulation methodology.

INTELLIGENT SURROGATE MODELS: FROM MODELING TO TRAINING

Modeling, as the fundamental activity in simulation research, involves projecting the real world onto a logically computable "problem space" through conceptual abstraction (primary modeling) and mathematical formalization (secondary modeling). The whole process is constrained in the framework of existing multidisciplinary knowledge systems. However, with the advancement of AI, data-driven methods are no longer merely the "calibrate" or "supplement" of the traditional physics-based models. The objective laws and complex relationships are usually captured by the high-dimensional latent spaces embedded inside the Intelligent Surrogate Models. Take Physics Informed neural networks(PINN) for example, from microscopic particle motion simulation to macroscopic weather forecasting, it consistently demonstrates the potential to surpass traditional numerical models in both accuracy and

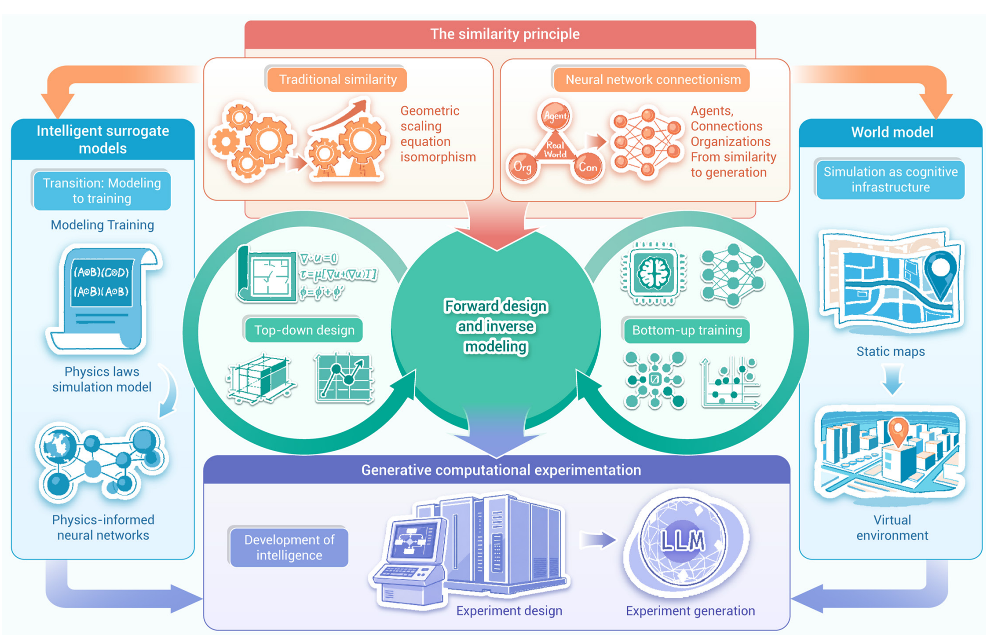

Figure 1. Conceptual framework of simulation intelligence.

efficiency. Thus, from first principles, Intelligent Surrogate Models, based on the artificial neural network, mark a fundamental shift in how we build the simulation system: From "Modeling" To "Training".

WORLD MODEL: INTELLIGENCE EMERGES THROUGH UNBOUNDED SIMULATION

The concept of the "World Model" originates from agent-centric researches such as reinforcement learning, aiming to construct an internal representation of environment dynamics. However, the role of the World Model has been confined to supporting an agent's decision-making within limited contextual boundaries, merely constructing a static version of world perceived. As referred to Karl Popper's Three Worlds theory, World Model belongs to the artificial world. It is believed that the activities such as climate change and human behaviors should also be considered in the World Model. The emergence of blockchain, distributed reasoning, and human–machine hybrid intelligence is transforming the World Model to be a dynamic, open, and evolvable simulation system. Consequently, it is increasingly recognized that machine intelligences such as embodied intelligence are trained in simulation-based World Models. Enabling richer scenario coverage and more robust agent responses, platforms such as Genesis, Cosmos, and Airsim are more and more popular in Sim2Real research. As a result, From the view of simulation discipline, especially in the embodied intelligence research, a consensus has emerged. is made: "Intelligence emerges through unbounded simulation."

GENERATIVE COMPUTATIONAL EXPERIMENTATION: THE DEVELOPMENT OF INTELLIGENCE

Computation Experiment was initially regarded as the third paradigm of scientific research, it employs the computer as an "artificial laboratory",[2] inferring systemic principles by controlling input variables and observing output responses. However, in the era of AI, the significance of computational experimentation has far surpassed its original function of "hypothesis verification", it becomes a mechanism for intelligence development. The ImageNet project led by Fei-Fei Li marked the beginning of data-driven intelligence growth.[3] Static pattern recognition is insufficient, dynamic environments and behavioral interactions are necessary for the development of intelligence. Consequently, simulation experiments have become the foundational infrastructure for AI training: within virtual worlds, agents can experience, trial-and-error, learn, and evolve. Today, from OpenAI's virtual reinforcement learning environments to Tesla's autonomous driving data engine, generative computational experimentation has emerged as an "incubation field" for intelligence development. With the advent of LLM, AI has acquired the capability to understand experimental objectives, formulate hypotheses, and autonomously generate experimental protocols. AI becomes a "collaborator" in the experimental process. Under this trend, generative computational experimentation represents the frontier of convergence between simulation and AI. Thus, computational experimentation is transforming from a tool for validating scientific theories into an ecosystem for developing intelligence.

FORWARD DESIGN AND INVERSE MODELING: THE SYSTEM ENGINEERING OF SIMULATION INTELLIGENCE

Conventional systems engineering follows a top-down, forward-design approach: objectives are defined, mechanistic models are built, and system behaviors are analyzed via simulation—a process driven by human intent and Newtonian presuppositions. AI introduces a complementary bottom-up, inverse modeling pathway: starting from observational data, system structure and behavior emerge through learning.

Though seemingly opposed, these two directions constitute a dialectical foundation for system design. Forward design embodies the rational principle of minimal energy dissipation, pursuing efficient, interpretable systems via concise mechanisms. Inverse modeling, by contrast, begins with raw data, allowing patterns and structures to self-organize through iterative algorithms—gradually approximating underlying truths and unknown laws.

Therefore, in the System Engineering of Simulation Intelligence, systems arise not from design alone, but from a dynamic, bidirectional optimization cycle. Human-derived rational frameworks help interpret behaviors emerging from data, while new patterns discovered in data challenge and enrich those frameworks, driving them toward higher-dimensional understanding.

CONCLUSION

Simulation is undergoing deep integration with AI. The proposed Simulation Intelligence paradigm synthesizes top-down and bottom-up approaches, enhancing not only simulation but also addressing fundamental challenges such as Interpretability, Verification & Validation (V&V), and Credibility.

- Interpretability, the future work must integrate PINNs and attention mechanisms to make the latent spaces of these models transparent;
- V&V, the generative outputs and robust testing against adversarial perturbations within the World Models are used to make traditional V&V methods evolve;
- Credibility, a "Human-in-the-Loop" framework and hybrid modeling approaches (combining forward design with inverse modeling) to maintain the credibility required for engineering and decision-making.

Looking ahead, we anticipate advances in explainable simulation for complex systems, simulation-based training for extreme scenarios, and adaptive platforms for innovative design. Specifically, Intelligent Surrogate Models have substantially enhanced capabilities in world scientific frontiers, such as climate change prediction. In alignment with national major demands, high-fidelity World Models are indispensable for decision support under uncertainty. Regarding public health, Generative Computational Experimentation accelerates drug discovery pipelines. Furthermore, the integration of Forward Design and Inverse Modeling drives innovation across the key economic sectors, exemplified by advancements in industrial digital twins and autonomous logistics. Collectively, these strides will catalyze a revolutionary convergence of simulation science and artificial intelligence.

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All authors contributed to the manuscript and approved the final version.

DECLARATION OF INTERESTS

The authors declare no competing interests.